# A Universal Quantitative Descriptor of Dispersion Interaction Potential

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## Abstract

London dispersion, universally attractive forces originating from fluctuating dipoles, is omnipresent in molecules. While its understanding has recently made tremendous progress, its general appreciation is still lagging behind electrostatics. This can be explained by the simple tools available to study electrostatic interactions like electrostatic potential (ESP) maps and partial charges and a lack thereof for dispersion. We herein report a universal quantitative descriptor of dispersion interaction potential, which allows assessing dispersion visually by London dispersion potential (LDP) maps, and quantitatively using the average LDP on the van der Waals (vdW) surface. We demonstrate the utility of these new tools by constructing a quantitative dispersion energy scale of the elements and common substituents, studying non-covalent interactions (NCIs) and developing modern linear free energy relationships in catalysis.

## Introduction

London dispersion is ubiquitous in molecular systems. On the one hand, they have long been well appreciated to explain bulk properties of matter,[1] on the other hand, they have been widely ignored to describe inter- and intramolecular interactions of solutes. However, in recent years, there was an upsurge of the appreciation of dispersion in small molecules in solution. Several studies addressed the concomitant compensation compared to the gas phase and found that dispersion is largely, but not fully, compensated.[2–8] Concurrently, the introduction of so-called DEDs was proposed as design principle to tune interactions in solution.[9–11] Consequently, this new paradigm, *inter alia*, was successfully applied to isolate stable hexaphenylethane derivatives having very long C-C bonds[6,7,10,12] and to guide the ligand design of CuH-catalyzed hydroamination reactions for increased reactivity.[13,14]

While DEDs find growing application, what is still missing is a universal scale to estimate the dispersion abilities of groups in a molecule and guide the rational design of dispersion-mediated reactivity, selectivity and interaction. Simply using molecular polarizabilities found limited application, presumably due to lack of general applicability as it disregards ionization potential and specific interactions.[6,15–17] Schneider estimated dispersion increments for various functional groups from binding affinity measurements of porphyrins with a variety of guest molecules in water.[18] However, it is not clear whether the increments are rather a measure of size as they correlated both with polarizabilities and surface areas. Additionally, Sigman proposed interaction parameters of substituted aromatic rings obtained from computed interaction energies and successfully applied them to predict stereoselectivity in a number of catalytic reactions.[19–21] Their main drawbacks are that they are quite expensive to compute, limited to aromatic systems and account for more than just dispersion. Recently, based on previous suggestions by Dunitz,[22] the so-called P parameter was introduced to quantify the dispersion ability of alkanes and perfluoroalkanes.[23] Despite promise as general parameter, its main limitation was the complicated procedure required to compute it. We herein report on the generalization of the previously proposed P parameter towards an easy to compute, universal and quantitative measure to assess dispersion interaction potential of molecules and on its application to various problems in chemistry.

## Results

**Methodology.** Starting from the London dispersion formula,[24] the P parameter was defined to describe the dispersion interaction energy between two atoms or groups of atoms (1 and 2) having a single contact as product of their P values:[23]

$$E_{disp}^{1,2} = -\frac{3}{2}\frac{I_1 I_2}{I_1 + I_2}\frac{\alpha_1 \alpha_2}{{R_{1,2}}^6} \approx -P_1 P_2 \quad (1)$$

$$P_i = A_i \frac{\alpha_i}{{R_{1,2}}^3} \; (i = 1, 2) \quad (2)$$

$I_1$ and $I_2$ are the ionization potentials of 1 and 2, $\alpha_1$ and $\alpha_2$ are the corresponding polarizabilities, $R_{1,2}$ is the distance between 1 and 2, and $A_1$ and $A_2$ are related to the respective ionization potentials. By comparing the London dispersion formula with atom-pairwise dispersion correction schemes,[25] where $C_n^{1,2}$ are heteroatomic dispersion coefficients, we realized that P could also be defined using homoatomic dispersion coefficients $C_n^{i,i}$:

$$E_{disp}^{1,2} = -\sum_n \frac{C_n^{1,2}}{{R_{1,2}}^n} \approx -P_1 P_2 \quad (3)$$

$$P_i = \sum_n \sqrt{\frac{C_n^{i,i}}{{R_{1,2}}^n}} \quad (4)$$

This new definition has two key advantages. First, the *ad-hoc* introduced pre-factor A is replaced with a well-defined physical quantity. Secondly, owing to the well-established dispersion correction schemes like TS,[26] XDM[27–30] or D3/D4,[31–34] $C_n$ coefficients can be computed readily and accurately for a wide range of elements. Hence, we could now test the potential of P as a general descriptor of dispersion interaction potential. We selected the recently developed D4 model[32,34] as our method of choice to describe dispersion accurately in a wide range of systems. In addition, we define the average P parameter of an atom or molecule with respect to its vdW surface (*i.e.* isosurface of electron density at 0.001 e Bohr$^{-3}$)[35] as $P_{int}$ to assess its LDP.

**Applications.** *1. Dispersion Scale.* First, we were interested to understand how $P_{int}$ changes in the free elements across the periodic table. While the periodic trends of the $C_n$ coefficients[31] and the atomic radii[36] are well-established, their interplay in the context of their LDP is not. Honoring the 150$^{th}$ anniversary of Mendeleev's discovery of the periodic table of the elements, we estimated $P_{int}$ for elements 1 – 86 and constructed a periodic table (Figure 1). Except for the alkali metals, $P_{int}$ does not change very much over the elements; all values are essentially within one order of magnitude. In addition, for the transition metals, $P_{int}$ is rather invariant within one group. For the main group elements, dispersion ability increases within a group when going down. Notably, the $P_{int}$ of the free elements does not necessarily correspond to the $P_{int}$ of atoms in molecules (Details in the SI).

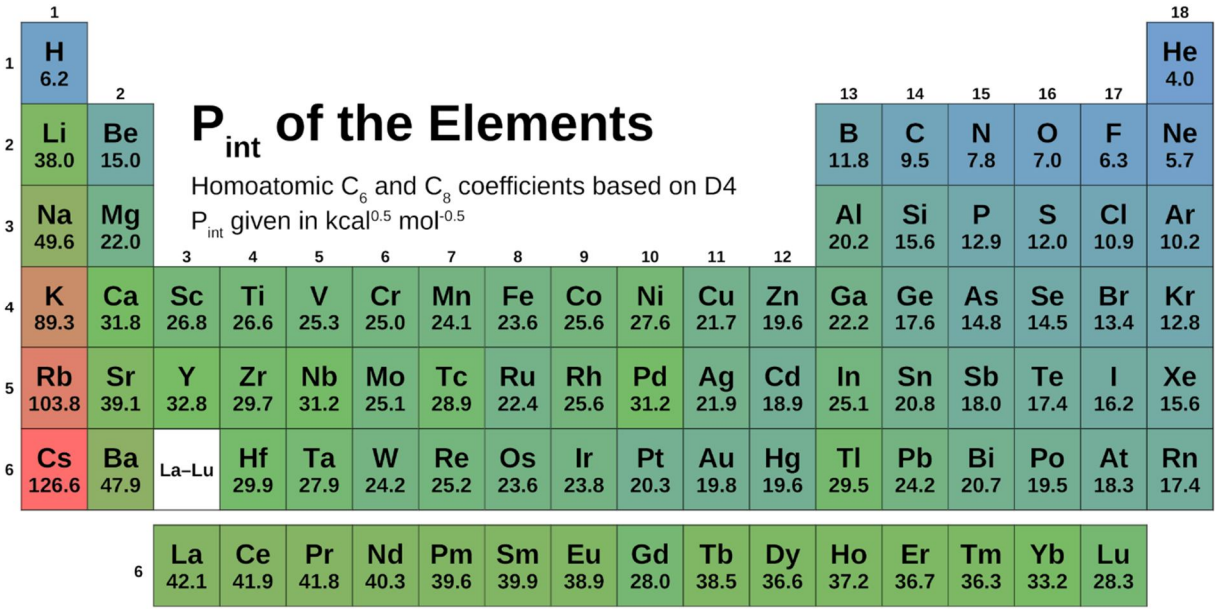



Figure 1. Calculated $P_{int}$ of the elements 1 – 86 arranged in a periodic table based on calculated atomic radii from the literature.[36]

Next, we wanted to rank common organic substituents according to their dispersion ability. Hence, we compiled a library and determined the average $P_{int}$, the maximum $P_{int}$ and the volume to assess both the dispersion ability of the groups and their steric demand. Additionally, we also included the product of $P_{int}$ and surface area ($A_{rel}$) to assess not only their dispersion ability in a single contact but also with respect to the maximum number of contacts. Table 1 contains 30 common substituents ordered by increasing $P_{int}$ and can be considered a quantitative DED scale. It shows that dispersion ability is somewhat correlated with number of atoms and size but not entirely. Introducing elements from higher periods like silicon, phosphorus and sulfur leads to increased dispersion ability. Notably, the product of $P_{int}$ and $A_{rel}$ shows a moderate correlation (F = 22) to the dispersion increments estimated by Schneider.[18]

Table 1. $P_{int}$, $P_{max}$, $V_{rel}$ (relative to Me) and the product of $P_{int}$ and $A_{rel}$ (relative to Me) of common organic substituents.

| Group | $P_{int}$ | $P_{max}$ [kcal$^{0.5}$ mol$^{-0.5}$] | $P_{int}$ $A_{rel}$ | $V_{rel}$ |
|---|---|---|---|---|
| -H | 3.6 | 6.2 | 1.5 | 0.29 |
| -F | 6.1 | 7.0 | 3.5 | 0.43 |
| -OH | 7.8 | 10.1 | 5.5 | 0.62 |
| -$NH_2$ | 8.7 | 12.0 | 7.4 | 0.81 |
| -CN | 9.6 | 11.0 | 10.0 | 1.03 |
| -Me | 9.8 | 12.5 | 9.8 | 1.00 |
| -$CF_3$ | 10.3 | 16.5 | 14.1 | 1.48 |
| -$NO_2$ | 10.4 | 15.2 | 12.5 | 1.24 |
| -OMe | 10.4 | 14.8 | 13.4 | 1.36 |
| -COOH | 10.9 | 15.4 | 14.4 | 1.41 |
| -$B(OH)_2$ | 10.9 | 15.6 | 16.1 | 1.62 |
| -$CONH_2$ | 11.3 | 15.9 | 16.3 | 1.60 |
| -Cl | 11.4 | 14.9 | 10.6 | 0.93 |
| -Et | 11.5 | 16.0 | 17.5 | 1.72 |
| -Ac | 11.6 | 17.2 | 18.4 | 1.80 |
| -$CF_2CF_3$ | 11.9 | 19.0 | 24.5 | 2.49 |
| -*i*Pr | 12.3 | 18.7 | 24.4 | 2.43 |

| | | | | |
|---|---|---|---|---|
| -SH | 12.3 | 17.4 | 13.5 | 1.18 |
| -*t*Bu | 12.9 | 18.4 | 30.6 | 3.13 |
| -$CF(CF_3)_2$ | 13.0 | 23.3 | 34.2 | 3.45 |
| -Br | 13.5 | 19.5 | 15.0 | 1.20 |
| -$SO_3H$ | 14.6 | 23.3 | 25.1 | 2.01 |
| -SeH | 14.6 | 22.2 | 18.3 | 1.39 |
| -TMS | 14.7 | 23.4 | 42.6 | 3.71 |
| -Cy | 14.7 | 20.4 | 42.5 | 4.01 |
| -$OPO_3H_2$ | 15.1 | 26.1 | 31.6 | 2.51 |
| -Ph | 15.3 | 23.3 | 38.6 | 3.30 |
| -OTf | 15.3 | 26.0 | 38.6 | 3.19 |
| -TIPS | 16.3 | 26.8 | 79.7 | 7.78 |
| -I | 16.3 | 25.1 | 22.0 | 1.57 |

*2. Dispersion Maps.* Next, we turned our attention to constructing LDP maps, which could be used analogously to ESP maps. For that, P needs to be computed on a 3-dimensional grid and visualized by projection onto isosurfaces of the electron density. The LDP of benzene is shown in Figure 2a. Local maxima on LDP maps of molecules indicate the strongest dispersion positions. Hence, they can be used to predict where a DED is strongest and would preferentially interact with another DED. To benchmark the results, we compared a sparse LDP map against a map of the dispersion component of the interaction of benzene with helium atoms placed at the same positions using SAPT (Figure 2b-c).[37] It can be seen that the LDP map computed using D4 and the benchmark map are identical with respect to their local extrema. Notably, the benchmark dispersion energy between a helium atom and benzene is 0.37 kcal $mol^{-1}$ at the global maximum and 0.17 kcal $mol^{-1}$ at the global minimum in the benchmark map. Additional benchmarks for LDP maps are provided in the SI.

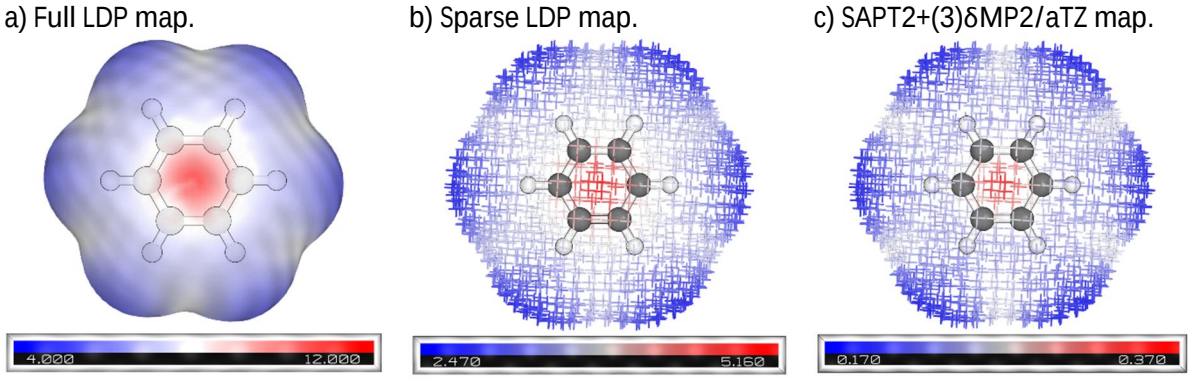



Figure 2. London dispersion potential map of benzene: a) Full LDP map from D4 (at $1 \cdot 10^{-4}$ e $Bohr^{-3}$, in $kcal^{0.5}$ $mol^{-0.5}$). b) Sparse LDP map from D4 (at $5 \cdot 10^{-6}$ e $Bohr^{-3}$, in $kcal^{0.5}$ $mol^{-0.5}$). c) Sparse map of the dispersion interaction energy component between He atoms and benzene (at $5 \cdot 10^{-6}$ e $Bohr^{-3}$, in kcal $mol^{-1}$).

In addition, intermolecular LDP maps can be constructed using Becke[38] surfaces to gauge the relative dispersion strength of particular interactions. The corresponding map for the T-shaped benzene dimer[39] is compared to an NCI plot[40,41] and to a dispersion interaction density (DID) plot,[42] which are well-established methods to visualize NCIs, in Figure 3. The LDP map correctly identifies the CH-π interaction as the strongest dispersion contribution. The main difference between the LDP map and the NCI plot is that the latter cannot distinguish between different types of NCIs; the LDP map only reveals dispersion. In addition, it is more straightforward to assess the relative interaction strengths from LDP maps. Notably, the dispersion energy between the two benzene molecules in the dimer was estimated to be 4.37 kcal $mol^{-1}$.[39]

a) LDP map on Becke surface. b) Intermolecular NCI plot. c) DID plot.

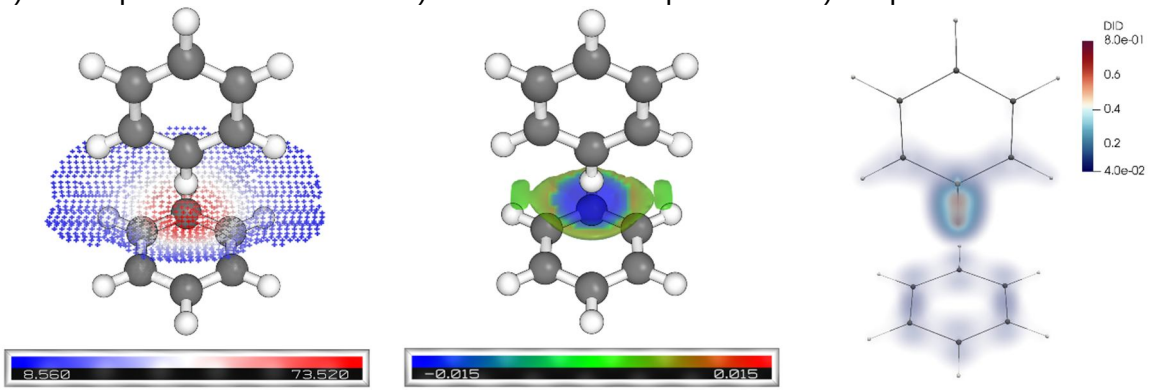



Figure 3. Visualization methods of NCIs in the T-shaped benzene dimer. a) LDP mapped onto the intermolecular Becke surface (values in kcal$^{0.5}$ mol$^{-0.5}$). b) Intermolecular NCI plot (values in au). c) DID plot (values in kJ mol$^{-1}$ Bohr$^{-3}$).

*3. Case Studies.* In this section, we apply the new tools to problems in various fields of chemistry.

*3.1 NCIs in Small Molecules.* First, we investigate ethene dimer, which is governed by dispersion.[43] To bring as many atoms as close together as possible, intuitively, one would predict a stacked structure, possibly with some displacement. However, looking at the LDP map, the maxima are not found on top of the π-system but rather to its sides (Figure 4a). This suggests that the sides prefer to get as close as possible. Hence, one would predict the most stable structure to have two interdigitated molecules of ethene. Indeed, high level computations find this structure to be the most stable conformer.[43] It is depicted in Figure 4b with an intermolecular LDP map illustrating the strong dispersion contacts. Notably, the corresponding total binding energy was estimated to be about 1.5 kcal mol$^{-1}$.[43]

a) LDP map of ethene. b) LDP map on Becke surface of ethene dimer.

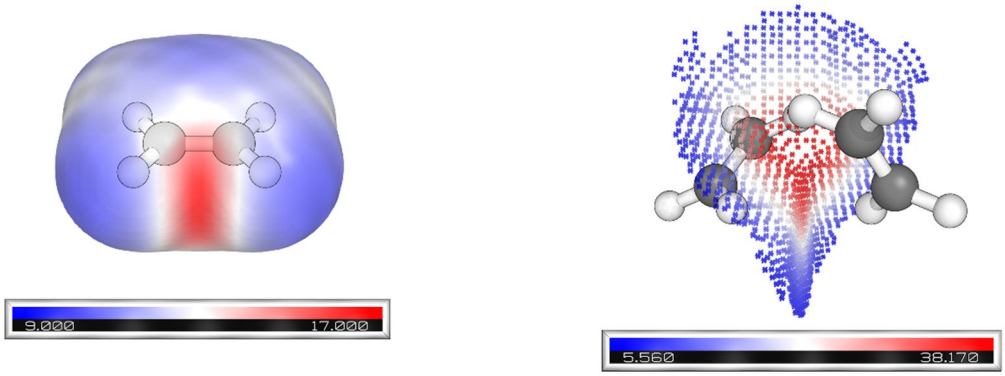
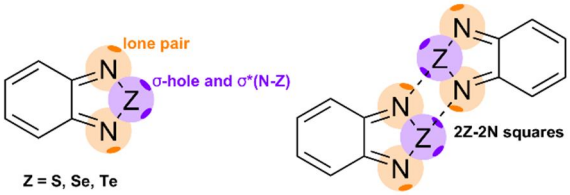



Figure 4. Investigation of the vdW dimer of ethene. a) Full LDP map from D4 (at 1 · 10$^{-3}$ e Bohr$^{-3}$). b) LDP mapped onto the Becke surface of the most stable dimer of ethene. Values are in kcal$^{0.5}$ mol$^{-0.5}$.

Another application is the study of chalcogen bonding. Depending on the type of chalcogen interaction at hand, electrostatics,[44] orbital interactions[45,46] or dispersion[44,47] can be dominant. Typically, orbital interactions are studied by various methods including NBO[48,49] and EDA-NOCV.[50] The method of choice to study the electrostatic component in these systems is the use of ESP maps revealing σ-holes.[51,52] In contrast, dispersion in these interactions is usually not given the same attention.[45,48–50,53] Hence, LDP maps could reveal additional insight. Recently, the chalcogen bonding in 2Z-2N squares was studied, where Z can be sulfur, selenium or tellurium (Scheme 1).[45,50,54–56]

Scheme 1. Chalcogen bonding in 2Z-2N squares (Z = S, Se, Te).




We computed the LDP maps of 2,1,3-benzothiadiazole, 2,1,3-benzoselenodiazole and 2,1,3-benzotellurodiazole (Figure 5). They reveal that there are local maxima of LDP between the chalcogen and nitrogen atoms. These maxima coincide with the σ-holes on the chalcogen atoms and the σ* orbitals of the N-S bonds. In addition, the trend in interaction energies of the corresponding dimers is parallel to the $P_{int}$ of the molecules or the local P values at the respective maxima. Thus, the strong electrostatic attraction is reinforced by dispersion making this motif a strong NCI. A similar coincidence of dispersion maxima and σ-holes was observed for halogen bonding.[57,58] LDP maps provide a means to study the spatial preference for dispersion in all systems with σ-holes revealing additional insight.

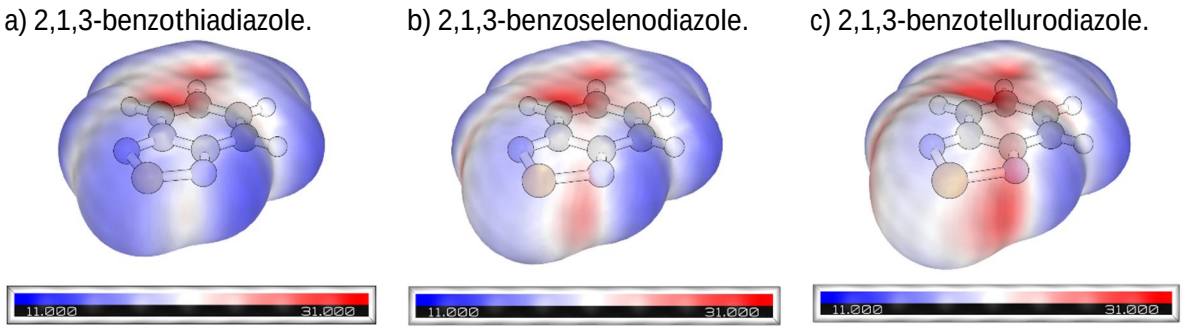
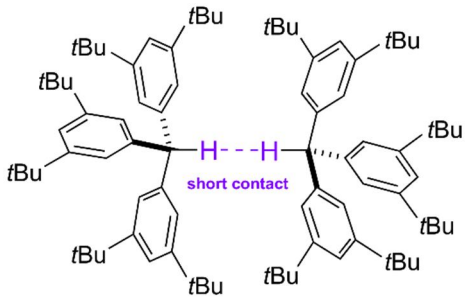



Figure 5. Investigation of chalcogen bonding in 2Z-2N squares (Z = S, Se, Te). Full LDP map from D4 (at $1 \cdot 10^{-3}$ e $Bohr^{-3}$) of 2,1,3-benzothiadiazole (a), 2,1,3-benzoselenodiazole (b) and 2,1,3-benzotellurodiazole (c). Values are in $kcal^{0.5}$ $mol^{-0.5}$.

Recently, an exceptionally short intermolecular H-H contact was observed in the crystal structure of tris(3,5-tert-butylphenyl)methane featuring dimers with face-on $Ar_3C$-H contacts,[59] which is still the shortest of its kind that is confirmed by neutron diffraction (Scheme 2).

Scheme 2. Short H-H contact in the crystal structure of tris(3,5-tert-butylphenyl)methane.




We computed the LDP map on the Becke surface of the corresponding dimer and compared it to a map of the normalized contact distance ($d_{norm}$) on the Becke surface,[60] the corresponding NCI plot and DID plot (Figure 6). While the $d_{norm}$ map shows that close contacts are distributed over the entire Becke surface, the LDP map reveals that close methyl contacts do not provide as much dispersion as the CH-π interactions, which is confirmed by the DID plot. In contrast, the relative strength of the contacts is harder to assess in the NCI plot as the CH-π interactions have both attractive and repulsive areas.

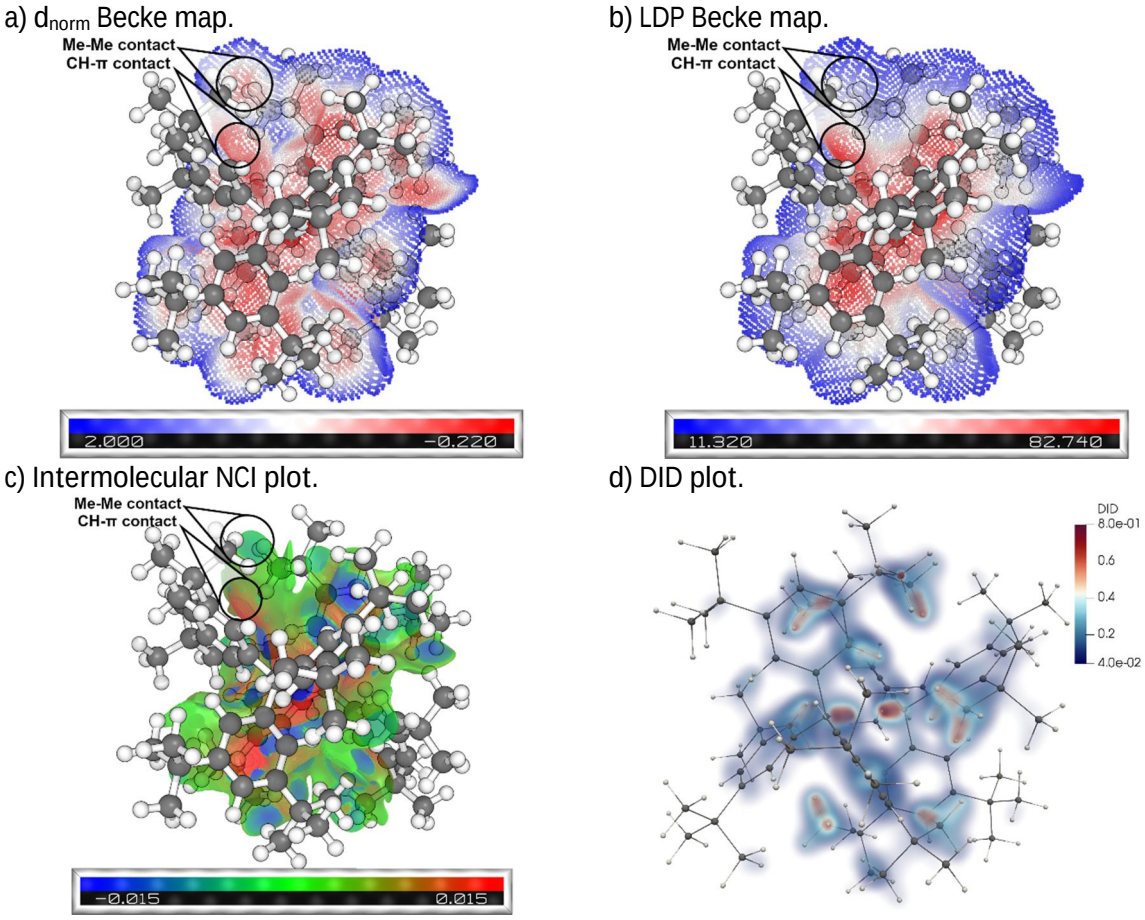



Figure 6. Investigation of tris(3,5-tert-butylphenyl)methane dimer using a $d_{norm}$ Becke map (a, values are dimensionless), an LDP Becke map (b, values in kcal$^{0.5}$ mol$^{-0.5}$), an intermolecular NCI plot (c, values in au) and a DID plot (d, values in kJ mol$^{-1}$ Bohr$^{-3}$).

*3.2 Spectroscopy.* Cryogenic spectroscopy allows isolation of weakly-bound complexes of molecules with so-called tag molecules, *i.e.* noble gases or small molecules like dinitrogen.[61–63] These complexes can be analyzed directly[64,65] or utilized for infrared photodissociation (IRPD) experiments.[66–70] In IRPD, the complexes are cleaved by absorption of photons, which can be recorded by photon intensity changes or by detection of the generated fragments. One main challenge in interpreting IRPD experiments is ascertaining the influence of the tag(s). The question where tags will bind was tackled recently by studying the stepwise cluster formation of pyrrole with dinitrogen, measuring the corresponding IR spectra and comparing them to computations.[65] The preferred binding sites were found to be the π-system and the N-H group;[65] they can be rationalized based on the ESP and LDP maps of pyrrole (

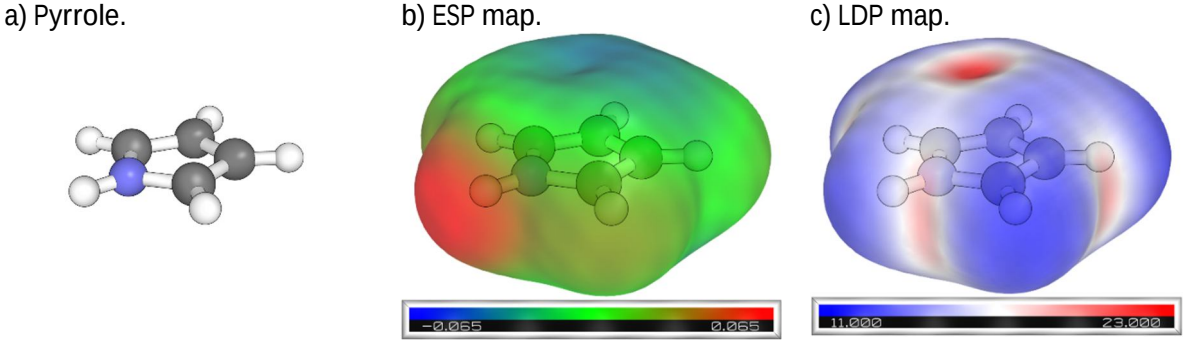


Figure 7). While the N-H group corresponds to the most positively polarized site, the π-system corresponds to the strongest dispersion site. Hence, this shows how ESP and LDP maps are complementary to predict preferred tag positions in weak complexes for cryogenic spectroscopy.

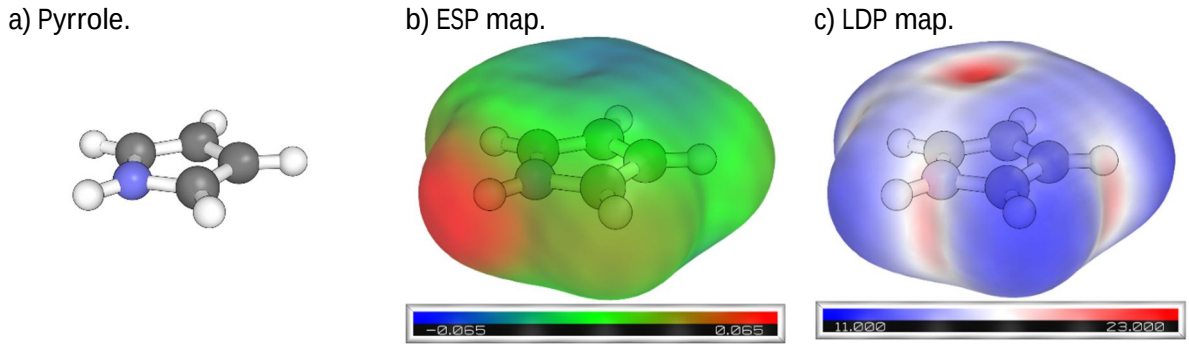



Figure 7. Investigation of preferred tag positions of pyrrole (a) using an ESP map (at $1 \cdot 10^{-3}$ e Bohr$^{-3}$, values in au) (b), and an LDP map from D4 (at $1 \cdot 10^{-3}$ e Bohr$^{-3}$, values in kcal$^{0.5}$ mol$^{-0.5}$) (c).

*3.3 Supramolecular Chemistry.* Next, we study hosts for single-walled carbon nanotubes and fullerenes. Despite their numerous applications, processing[71] and purifying[72] these materials is still a challenge. A successful strategy is using selective hosts for carbon nanotubes and fullerenes.[73] Small molecules with concave π-systems show great promise for selective binding.[73–75] Their dominant binding mechanism is dispersion with additional electrostatic contributions.[76] Corannulene is a popular motif for selective binding to fullerenes.[73] Its center is the preferential binding site for $C_{60}$ and $C_{70}$ fullerenes, which cannot be solely explained by maximizing contact area.[73,77] Hence, we studied the LDP map of corannulene to understand this peculiar preference (Figure 8). It can be seen that the dispersion maximum lies on the concave face. The respective $P_{max}$ equals 41 kcal$^{0.5}$ mol$^{-0.5}$, on the convex face $P_{max}$ is only 30 kcal$^{0.5}$ mol$^{-0.5}$. Hence, shape alone accounts for the significant difference in dispersion ability explaining the effectiveness of curved molecules for binding carbon nanotubes and fullerenes. In addition, LDP maps could serve as tools to design more effective hosts for carbon nanomaterials.

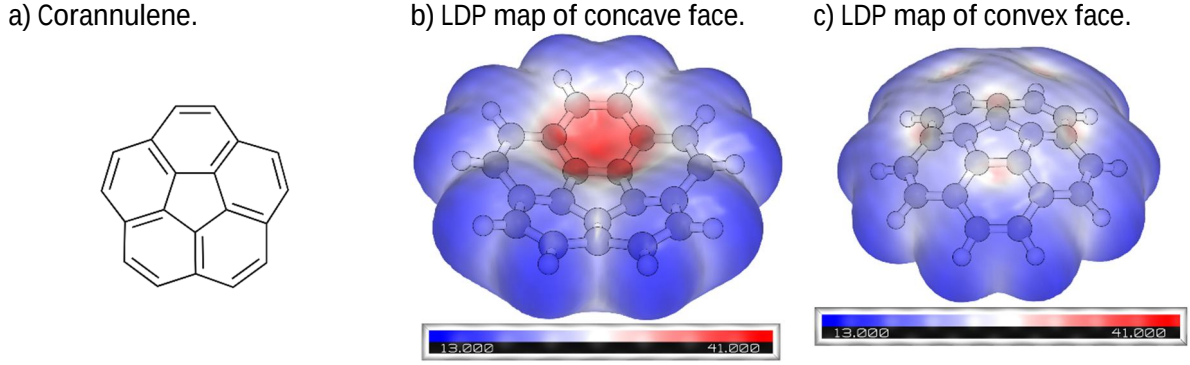
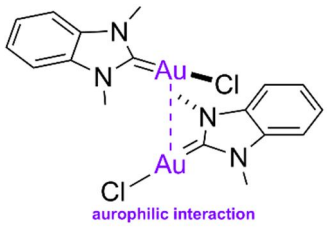



Figure 8. Investigation of LDP of corannulene (a) using LDP maps from D4 (at $1 \cdot 10^{-3}$ e Bohr$^{-3}$) viewed at from the concave (b) and convex (c) face. Values are in kcal$^{0.5}$ mol$^{-0.5}$.

*3.4 Organometallic Chemistry.* Next, we applied LDP maps to the study of metallophilic interactions.[78] The term "metallophilic" was coined to describe the attraction between two closed-shell metal cations,[78] and was rationalized by electron correlation effects attributed to dispersion.[78–82] Recent studies suggest that the contribution of the Au-Au contact is 3 – 8 kcal mol$^{-1}$ and that there is typically a significant ligand contribution as well.[83,84] Recently, several dimers of Au(I)-carbene complexes with aurophilic interactions were studied with local correlation methods.[85,86] Ligand-ligand interactions were found larger than aurophilic contacts.[85,86] We reinvestigated these findings with an LDP map of one of the Au(I)-carbenes (Figure 9). It shows that the maximum of dispersion is not on gold but on the

ligand, which has a large region of strong LDP. Hence, the LDP map confirms the previous results and shows that it can be used to understand the dispersion component of metallophilic interactions.

a) Aurophilic interaction in Au(I)-carbene.




b) LDP map of Au(I) carbene.

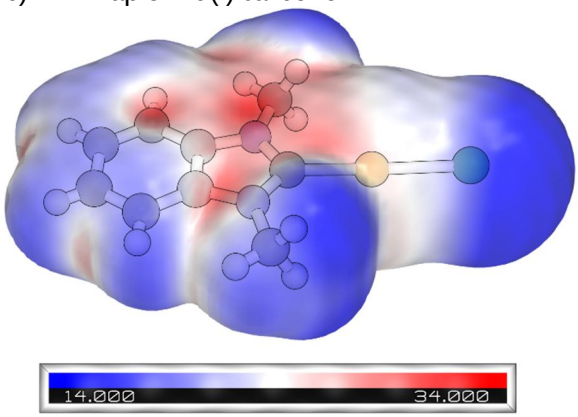
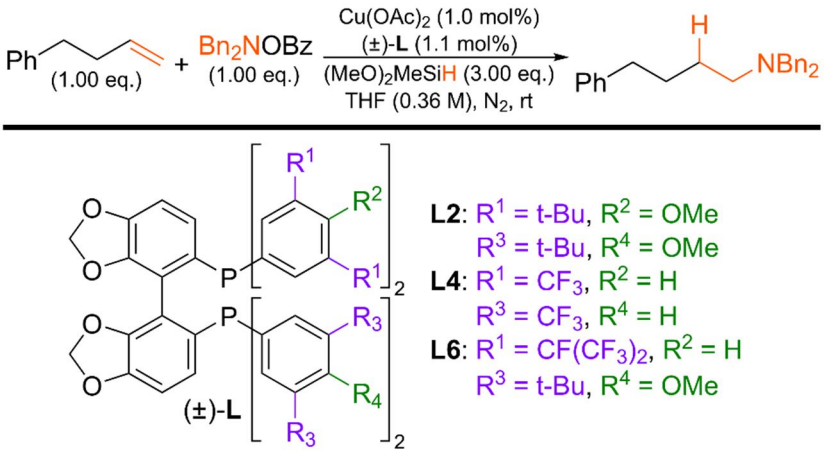



Figure 9. Investigation of aurophilic interactions (a) in a Au(I)-carbene complex using an LDP map (b) from D4 (at $1 \cdot 10^{-3}$ e $Bohr^{-3}$). Values are in $kcal^{0.5}$ $mol^{-0.5}$.

*3.5 Catalysis.* Recently, Buchwald and Liu studied CuH-catalyzed hydroamination reactions of alkenes (Scheme 3).[13,14]

Scheme 3. CuH-catalyzed hydroamination of alkenes and subset of ligands employed.




They proposed a ligand-substrate interaction model to establish the importance of dispersion in the hydrocupration transition state (TS) and correlated the through-space interactions of various ligands to their reactivity.[13] They applied this model for computationally guided ligand design and managed to develop a new best-performing ligand by retaining stabilizing dispersion and increasing through-bond stabilization by electronic modification.[14] We want to highlight how LDP maps and $P_{int}$ values could facilitate dispersion-oriented ligand design. First, we correlated the $P_{int}$ value of the aryl substituents on the bidentate phosphines against the ligand-substrate dispersion in the hydrocupration TS ($\Delta E_{disp}$, Figure 10).

a) Correlation of $\Delta E_{disp}$ against $P_{int}$(Ar).

b) Definition of $P_{int}$(Ar) in bidentate phosphines.

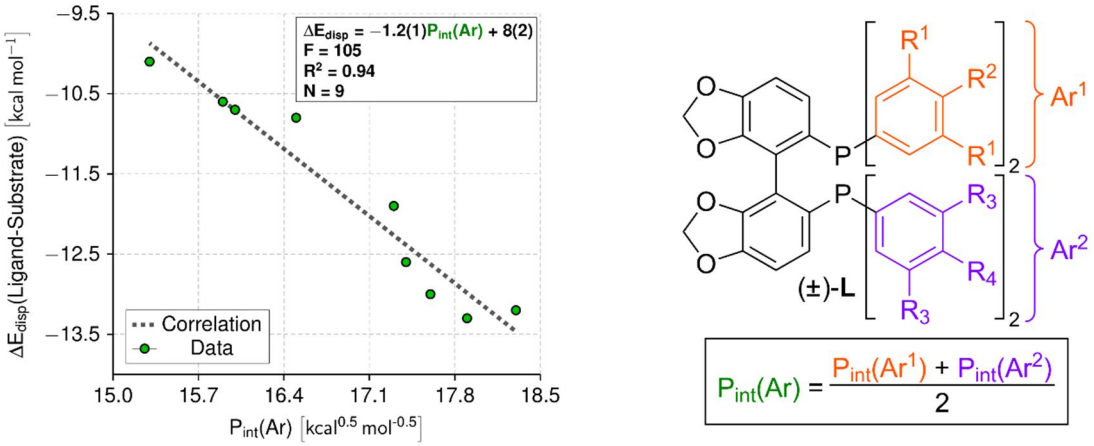
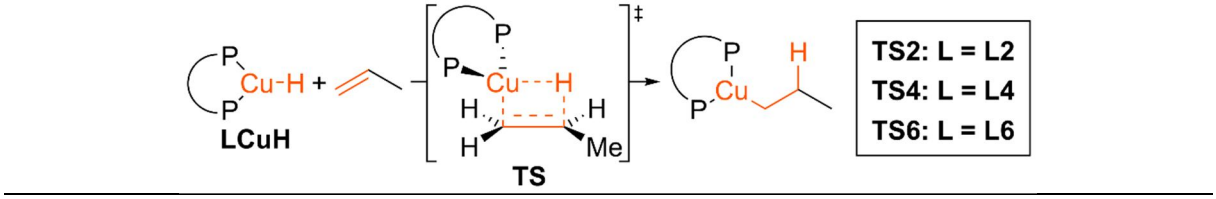



Figure 10. Correlation of ligand-substrate dispersion in the hydrocupration TS (a) against $P_{int}$ of the aryl groups in bidentate phosphines (b) in the CuH-catalyzed hydroamination of alkenes.

The good correlation suggests that the through-space dispersion can be estimated using the $P_{int}$ of the aryls alone. Notably, computing $P_{int}$ is much cheaper and, hence, greatly facilitates ligand optimization. In addition, tert-butyl was substituted for perfluoro-isopropyl groups and comparable dispersion was observed.[14] These groups have almost the same $P_{int}$ value showing that they should indeed lead to similar dispersion (Table 1). Furthermore, we also visualized the ligand-substrate dispersion using LDP Becke maps in the TSs (Figure 11). While TS4 has a significantly reduced ligand-substrate dispersion, both TS2 and TS6 show comparable interactions. Figure 11 can be used to assess where dispersion would have the strongest impact.



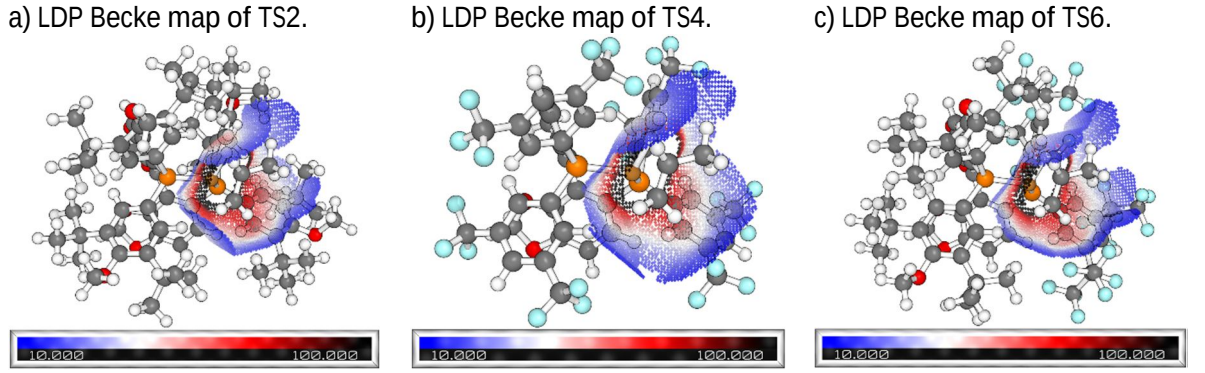
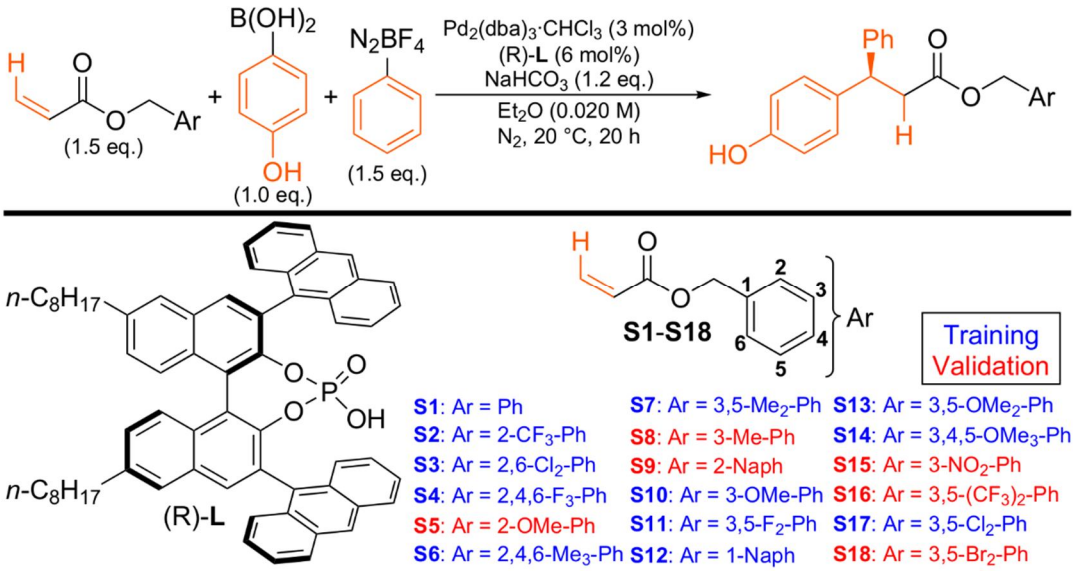




Figure 11. Investigation of ligand-substrate dispersion in the hydrocupration TS of CuH-catalyzed hydroamination reactions of alkenes using LDP Becke maps (a-c). Values are in kcal$^{0.5}$ mol$^{-0.5}$.

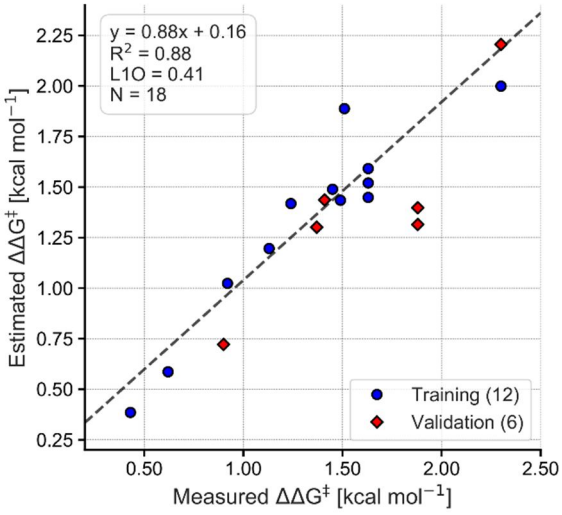
Recently, Sigman introduced computed interaction energies and distances as parameters for NCIs between aromatic rings[19] and applied them successfully to several case studies.[19–21] We wanted to test whether $P_{int}$ could replace Sigman's energy parameters, which he termed Eπ,[19] for the same type of MLFER analysis. Hence, we reanalyzed the data of the Pd-catalyzed enantioselective 1,1-diarylation of benzyl acrylates with varying benzyl groups (Scheme 4).[20,87] Simply replacing $^{S}$Eπ with either $P_{int}$ or the product of $P_{int}$ and $A_{rel}$ resulted in models comparable in quality to the original one (Figure 12).

Scheme 4. Conditions of Pd-catalyzed enantioselective 1,1-diarylation of benzyl acrylates together with the acrylates employed for the MLFER model.




a) MLFER analysis using $P_{int}$.

$\Delta\Delta G^{\ddagger} = 0.63P_{int} - 10.53NBO_{C1} + 11.12P_{int}NBO_{C1}$




b) MLFER analysis using $P_{int}A_{rel}$.

$\Delta\Delta G^{\ddagger} = 0.84P_{int}A_{rel} - 2.98NBO_{C1} + 3.62P_{int}A_{rel}NBO_{C1}$

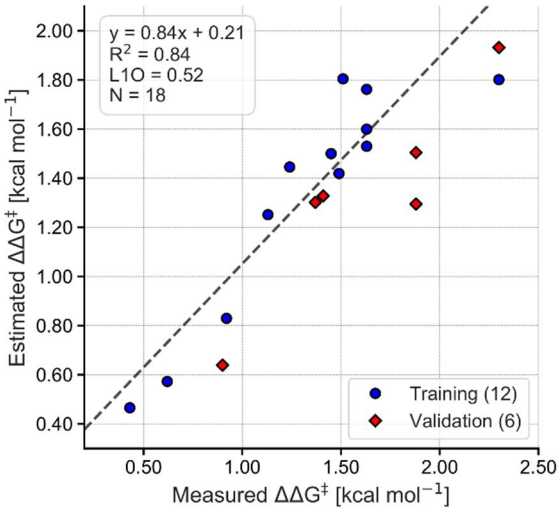



Figure 12. MLFER analysis of Pd-catalyzed enantioselective 1,1-diarylation of benzyl acrylates using $P_{int}$ (a) and the product of $P_{int}$ and $A_{rel}$ (b) to replace $^{S}E\pi$ from the original model.

Using only $A_{rel}$ resulted in a model of lower quality. Additionally, **S4** was a significant outlier in the original model and therefore disregarded.[20] In our models, we included **S4** in the training set and did not observe it as an outlier. Notably, the product of $P_{int}$ or $P_{int}A_{rel}$ and $NBO_{C1}$ result in significant single parameter correlations ($R^2 = 0.63$ and 0.64, respectively). Overall, we demonstrated that LDP maps and $P_{int}$ can facilitate catalyst design and help to understand the role of dispersion.

## Discussion

**Methodology.** The definition of P relies on methods providing access to $C_n$ dispersion coefficients. In principle, the Tkatchenko–Scheffler[26] (TS) dispersion model, the exchange-dipole moment[27–30,88] (XDM) dispersion model or the D3[31] or D4[32] model could be employed for that purpose illustrating the flexibility of our approach.[25,89] Within this work, we tested XDM, D3 and D4 and found that all

these models yield comparable results for a wide range of molecules. However, D4 provides the most accurate $C_n$ coefficients of all these approaches[32] and, hence, it was our method of choice. D4 is only slightly more expensive than D3 and cheaper than XDM and, therefore, best in terms of cost benefit ratio. There are several assumptions inherent in the new definition of P. First, we are only using homoatomic dispersion coefficients because the interaction partner is undefined. When P values are used to estimate dispersion energies between two fragments, this results in using the geometric mean of two homoatomic dispersion coefficients to appxorimate the heteroatomic one. This approach was already used in the D2 correction as a good approximation of exact Casimir–Polder integration.[25,90] Hence, this approximation is not only convenient but also justified.

Moreover, our current P measure neglects many-body dispersion. This leads to a disregard of part of the anisotropy. While the Axilrod–Teller–Muto term[91,92] could be used to estimate this contribution, it is only important in large molecules[93,94] and its contribution typically amounts to less than 5 %.[25] In addition, to implement it, additional approximations would be necessary and, thus, we decided to neglect it. Overall, despite the approximations inherent in our definition of P, our benchmarking indicates that P is a good quantitative descriptor of LDP. This is corroborated by the comparison of LDP maps using P with the corresponding dispersion interaction maps based on SAPT[95–98] and LED-DLPNO-CCSD(T) (Details in the SI).[99,100]

Notably, we implicitly account for a large portion of the dispersion anisotropy when using molecular surfaces based on electron density to compute LDP maps and $P_{int}$ values. The reason for that is polar flattening,[101,102] which leads to anisotropy in the local vdW radii, which in turn introduces anisotropy to the local P values.[58] It was shown previously that polar flattening combined with isotropic atom-centered dispersion corrections like D3 can reproduce the anisotropy of intermolecular interactions in BrF, BrCl and $Br_2$ predicted by higher levels of theory surprisingly well.[58] Notably, it introduces anisotropy only to the repulsive component.[58] We compared the LDP map of bromine to benchmark interaction surfaces and found the local extrema to be well reproduced (Details in the SI).[58] This illustrates that LDP maps on isosurfaces of electron densities are a simple tool to study the anisotropy of dispersion in molecules at least in a semi-quantitative manner.

Finally, $P_{int}$ values are rather large, especially when compared to dispersion energies between single atoms at equilibrium distances,[103] which are typically $10^{-1}$ – $10^{1}$ kcal mol$^{-1}$. The main reason is that we use vdW radii as interaction distances. However, for intermolecular interactions, they are too small as the size of the interaction partner is unaccounted for. In homoatomic interactions, the interaction distance is about twice the size of the vdW radii, which leads to a reduction in $P_{int}$ by a factor of 8 to 16, *i.e.* about one order of magnitude. This correction factor brings the estimated homoatomic interaction energy obtained by multiplying two P values to the correct order of magnitude.

**Applications.** We introduced LDP maps to have a tool akin to ESP maps available for dispersion. They provide a new means to visualize dispersion because they rely on a different approach compared to existing methods like NCI plots or DID plots. NCI plots reveal regions of attractive and repulsive interactions in molecular complexes but they cannot distinguish dispersion from other components.[40–42] DID plots reveal the origin and relative strength of dispersion interactions in molecular complexes.[42] Hence, they can only be applied to study existing interactions. In contrast, LDP maps reveal where new dispersion interactions would be strongest. Therefore, they are complementary to both NCI and DID plots. We also showed that LDP maps can be projected onto Becke surfaces of molecular complexes

to reveal the relative strength of existing dispersion interactions. They provide similar information as NCI plots with the difference that they only indicate dispersion.

Moreover, we established a fast computational procedure for computing P parameters of molecules starting from SMILES[104–106] making use of Open Babel[107] for 3D structure generation, GFN2-xTB[108,109] for extensive conformer search and structure optimization and DFT densities at the PBE[110]/def2-SVPD[111,112] level of theory. This computationally cheap approach makes it possible to compute $P_{int}$ for molecules with up to 100 atoms and more within minutes to a few hours on a single core on a desktop PC at the time of publication. The bottleneck is the extensive conformer search despite relying on semi-empirical methods. Overall, this makes $P_{int}$ very attractive for correlation analysis as the computational cost is in between traditional 2D and 3D quantitative structure–activity relationship (QSAR) parameters and modern physical organic parameters.[17] Notably, $P_{int}$ is orders of magnitude faster to compute than the Eπ parameters.[19] Additionally, $P_{int}$ is not limited to aromatic rings and can be applied to any dispersion interaction.

With respect to potential applications, LDP could be used to treat dispersion in continuum solvation models in a less empirical way. Solute-solvent dispersion could be estimated from the contact of the local solute P with the average solvent P. It needs to be tested whether this can be a feasible approach. We also envision potential applications in fragrance chemistry. The understanding of the mechanism of olfaction is still very limited.[113–115] Structure–odor relationships using QSAR parameters are a common tool to predict what molecules smell like[113] and machine learning is emerging as promising new method to predict odor class and intensity.[115] LDP densities could be used as multidimensional dispersion descriptors adding a new dimension to the variety of descriptors already applied.

## Conclusions

In this work, we redefined the dispersion interaction potential P making use of the widely employed $C_n$ dispersion coefficients and established the average LDP on the vdW surface, which we term $P_{int}$, as descriptor of LDP of an atom or molecule. We also introduced LDP maps as visual tool to understand where new dispersion contacts would be most attractive. Using these tools, we looked at trends of dispersion in the periodic table, established a quantitative DED scale of common organic substituents and applied them to common problems dealing with dispersion interactions in various fields. Their simple computation and broad applicability make these tools very attractive to tackle various chemical problems and we envision large potential for many future applications.

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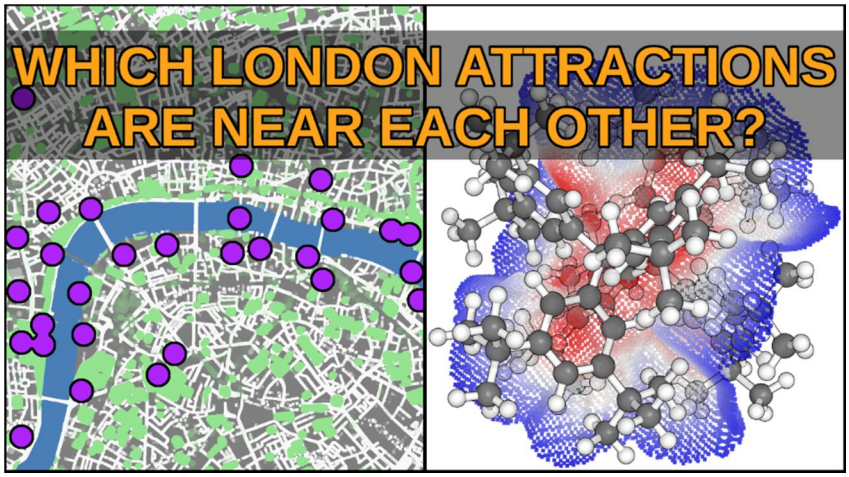



A Map of London: A new descriptor of quantitative dispersion interaction potential was introduced and applied to the study of non-covalent interactions in spectroscopy, nanomaterials and catalysis. It allows the generation of London dispersion potential maps indicating the site of strongest dispersion and the estimation of average dispersion interaction strength of any atom or molecule.

**Keywords:** dispersion forces, non-covalent interactions, molecular recognition, interaction descriptors, interaction maps, correlation analysis

# Contents

# 1 Computational Methods

In this section, we will describe the computational methods in detail. The following programs were employed for all the computations in this study:

- Orca (version 4.1.0)[1,2]
- molden2aim (version 4.2.1)[3]
- dftd3 (version 3.1 Rev 1)[4]
- dftd4 (version 2.0)[5,6]
- xtb (version 6.1 beta)[7,8]
- crest (version 2.5.1)[9,10]
- Multiwfn (version 3.6)[11]
- PSI4 (version 1.2)[12,13]
- ADF (version 2016)[14]
- Gaussian (version 09, revision D.01)[15]
- postg[16,17]
- IGMPlot (version 2.4.2)[18–21]
- Molpro (version 2015.1.18)[22]
- PyMol (version 1.8.4)[23]
- Paraview (version 5.6.0)[24,25]
- Python (version 3.6.8)[26]

Orca (version 4.1.0)[1,2] was employed for all density functional theory (DFT) calculations except for some of the benchmark dispersion map calculations. Density-fitting (also called resolution of identity, RI)[27–29] was employed using the RI-J approximation to speed up self-consistent field (SCF) calculations using the "def2/J" auxiliary basis set. Unless noted otherwise, "Grid5" was used in conjunction with "NoFinalGrid". Geometry optimizations for small molecules were carried out using the PBE[30]/def2-TZVP[31] with the "TightOPT" keyword. Other geometries were taken directly from the literature, either from crystal struc-

tures or from computations. All geometries are provided in a ZIP archive as additional supporting information material.

P parameters of functional groups were computed as follows. The functional groups were attached to an ethynyl group. The lowest energy conformers of the respective molecules were found using crest (version 2.5.1)[9,10] using the MTD-GC workflow with default settings at the GFN2-xTB[7,8] level of theory. The electron density was obtained either from PBE/def2-SVPD[32] single point calculations (Orca keywords: RI, def2/J, NormalSCF, Grid4, NoFinalGrid) or from Multiwfn (version 3.6)[11] as promolecular electron density. The van der Waals (vdW) surface was obtained using Multiwfn (version 3.6)[11] based on the respective density with isovalues of 0.00100 (for PBE/def2-SVPD densities) or 0.00174 (for promolecular densities, isovalue optimized to reproduce vdW volume of ethene from PBE/def2-SVPD densities). The spacing between points was 0.25 Bohr. The points of the vdW surface corresponding to the ethynyl group were removed and the dispersion coefficients of the ethynyl group were not included in the computation of the P values. For the remaining points, the P parameter in each point was calculated as defined in the main manuscript. For dispersion coefficients, dftd3 (D3), dftd4 (D4) or postg (XDM) were used. The volume and surface area were determined by taking the total volume and surface area of the molecule and removing the volume and surface area of the ethynyl group, which were determined as half the volume and surface area of buta-1,3-diyne, respectively. All volumes and surface areas were determined as ratios with respect to the methyl group.

LDP maps of molecules were computed as follows. The electron density was obtained from PBE/def2-TZVP single points calculations (Orca keywords: RI, def2/J, Grid4, NoFinalGrid). Density cube files were generated using Multiwfn (version 3.6).[11] P parameters were computed in all points of the cube file. For dispersion coefficients, dftd3 (D3), dftd4 (D4) or postg (XDM) were used. LDP maps were visualized using PyMol (version 1.8.4).[23]

Benchmark dispersion maps were computed as follows. Noble gas atoms were placed systematically across the molecular surface of the respective molecules. The positions were

determined based on PBE/def2-TZVP densities using Multiwfn (version 3.6)[11] by generating isosurfaces of electron density with isovalues of 0.000005 for He, 0.000001 for Ne and 0.0000005 for Ar, and with a spacing between points of 1.1 Bohr for He and 1.2 Bohr for Ne and Ar. The isovalues were chosen based on SAPT2+(3)δMP2 calculations in order to have overall attractive interaction energies. Typically, this resulted in $10^2$ – $10^3$ points on the molecular surface. The dispersion energy was either determined directly by energy decomposition analysis methods between the molecules and the respective noble gas atom or as energy difference between the dispersion corrections for the molecules with and without noble gas atom. The following table lists the methods used to determine the dispersion between the molecules and the noble gas atoms together with the corresponding basis sets employed, programs used and additional computational details.

| **Method** | **Basis set** | **Software** | **Comments** |
|---|---|---|---|
| sSAPT0[33] | jun-cc-pVDZ[34,35] | PSI4 | The RI-JK[36] approximation for HF calculations was used with the jun-cc-pVDZ/JK[37] fitting basis set. |
| SAPT2+[33] | aug-cc-pVDZ[38] | PSI4 | The RI-JK[36] approximation for HF calculations was used with the aug-cc-pVDZ/JK[36] fitting basis set. |
| SAPT2+(3)δMP2[33] | aug-cc-pVTZ[38] | PSI4 | The RI-JK[36] approximation for HF calculations was used with the aug-cc-pVTZ/JK[36] fitting basis set. |
| LED[39]-DLPNO-CCSD(T)[40,41] | cc-pVQZ[42] | Orca | The RI-JK[36] approximation for HF calculations was used with the cc-pVQZ/JK[36] fitting basis set. TightPNO[43] thresholds were used. |
| B3LYP[44–46]-D3(BJ,abc)[4] | – | dftd3 | – |
| B3LYP[44–46]-D4(BJ,abc)[5,6] | – | dftd4 | – |
| B3LYP[44–46]-NL[47,48] | def2-QZVP[31] | Orca | The RIJCOSX[49,50] approximation with the def2/J[51] fitting basis set was used. |

| Method | Basis set | Software | Comments |
|---|---|---|---|
| B3LYP[44–46]-dDsC[52–54] | QZ4P[55] | ADF | Density fitting was performed using the RI approximation[55,56] with the QZ4P[55] fitting basis set. |
| B3LYP[44–46]-XDM[57–61] | aug-cc-pVTZ[38] | Gaussian, postg | – |

For non-covalent interaction (NCI) plots, reduced density gradient (RDG) isosurfaces (isovalue of 0.75) of intermolecular complexes were generated using IGMPlot[18–21] and visualized using PyMOL (version 1.8.4).[23] Geometries were taken from the literature. Densities were obtained from promolecular estimates. All interactions with at least a fraction of 0.90 of the density from only one of the two fragments were turned off so that only intermolecular interactions were visualized.

Dispersion interaction density (DID)[62] plots were generated using Molpro (version 2015.1.18)[22] by SCS-LMP2[63,64]/aug'-cc-pVTZ[38,42] calculations making use of the RI-JK[36] approximation for the HF step with the automatically generated JKFIT basis set. Notably, the aug'-cc-pVTZ uses diffuse functions only for non-hydrogen atoms. Localization was carried out using Pipek-Mezey orbitals and visualization was conducted in Paraview.[24,25] Geometries were taken from the literature.

Multiple linear regressions were carried out using Python (version 3.6.8)[26] using the scikit-learn package (also called sklearn, version 0.20.2).[65] Target values and parameters, except for $P_{int}$ and $A_{rel}$, were taken from the respective literature reports. Both the parameters and target values were normalized before data analysis. Linear regression was carried out using `sklearn.linear_model.LinearRegression`. Leave-one-out cross validation was performed using `sklearn.model_selection.LeaveOneOut`.

Atomic P parameters from hydrides and fluorides of the main group elements were determined as follows. The number of hydrogen and fluorine atoms bound to the central element

were chosen to satisfy the octet rule. Geometries were optimized at the TPSS[66]/def2-QZVP level of theory (Orca keywords: RI, def2/J, TightOpt, Grid5, NoFinalGrid). Subsequent single point calculations were carried out at the DKH2[67,68]-TPSS/ANO-RCC-QZP[69] level of theory (Orca keywords: RI, AutoAux, NoFrozenCore, TightSCF) and were used to obtain electron densities. The vdW surface was obtained using Multiwfn (version 3.6)[11] with isovalues of 0.00100 and a spacing between points of 0.25 Bohr. Consecutively, the P parameter effected solely by the central element was calculated for all the points on the vdW surface. The maximum P value on the vdW surface was used as atomic P parameter.

# 2 Supplementary Results and Discussion

In this section, additional results, that did not fit into the main manuscript, are presented and discussed.

## 2.1 Applications

### 2.1.1 Dispersion Scale

The presence of bonds and electronegativity differences between bonded atoms affects both size and $C_n$ coefficients. Hence, the net effect on $P_{int}$ is not straightforward. We assessed that by investigating both hydrides and fluorides of the main group elements (until Rn, except for the noble gases) and determined the corresponding $P_{int}$ effected by the elements alone. Typically, changes can be very significant but far less than the total range of values observed in the free atoms. For instance, in $CH_4$, the $P_{int}$ of carbon decreases to 7.6 and the $P_{int}$ of hydrogen decreases to 4.9. In $CF_4$, the $P_{int}$ of carbon decreases to 6.4 and the $P_{int}$ of fluorine increases to 7.3. Table S1 compares the corresponding results. The biggest effect is observed for lithium. The $P_{int}$ of lithium in LiH and LiF increases significantly relative to the atomic value. The main reason for that is that the size difference between atomic lithium and lithium in the molecules dominates over the significant decrease in dispersion coefficients. The same effect is observed for sodium but less pronounced. On the contrary, for potassium, rubidium and cesium, the $P_{int}$ of the hydrides and fluorides is significantly lower than in the free atoms. Generally, for most of the other elements, the influence of the presence of bonds and the electronic environment is significantly smaller showing that the $P_{int}$ of the free atoms is a good first approximation to gauge their dispersive potential. The changes in $P_{int}$ tend to be bigger for less electronegative elements illustrated by aluminium more than doubling the $P_{int}$ when going to fluoride or by polonium doubling the $P_{int}$ when going from atomic Po to $PoF_2$. In general, most elements show an increase in $P_{int}$ when going from free atom to hydride or fluoride. Only carbon, potassium, rubidium and cesium show a decrease

in $P_{int}$ for both the hydrides and the fluorides. This suggests that while bonding decreases dispersion coefficients, the respective decrease in size of the atoms typically results overall in an increase of dispersive potential. This finding deserves more detailed investigations, which are outside the scope of this work and currently underway. However, it shows that the introduction of P as parameter to gauge dispersive potential provides new chemical insight.

Next, we looked more closely into the common substituents in organic chemistry already discussed in the main text (see Table 1). We computed the P parameters for several additional substituents. The corresponding results together with all the values already shown in the main text are provided in Table S2. The most dispersive group from the selected ones is the triphenylsilyl (TPS) group. It is most dispersive both with respect to average dispersive strength and single strongest dispersive contact. Additionally, it is also the group with the largest volume and surface area. Since it is relatively simple to introduce synthetically and is relatively inert under many reaction conditions, it might be an attractive choice as a single group providing a large amount of dispersion. Furthermore, we compared the $P_{int}$ of all the substituents using different computational approaches. We compared values based on both D3 and D4 dispersion corrections and with both PBE densities and promolecular densities. The corresponding results are given in Table S3. It can be seen that the D3 correction significantly underestimates the dispersive abilities of perfluoroalkyl groups compared to the D4 correction.[70] In addition, D3 also tends to underestimate the dispersive ability of groups with elements from the third row onward. The reason for that is that it does not properly account for redistribution of polarizability due to the electronic environment in these groups.[5] Using promolecular densities results in quite significantly different values. The correlation coefficients between the $P_{int}$ from PBE densities and from promolecular densities are 0.82 and 0.80 for D4 and D3, respectively. This demonstrates that accounting for the actual electronic environment of the atoms is crucial for the accurate estimation of the dispersive abilities of the substituents. It also suggests that substituent dispersion parameters based on promolecular densities should not be employed for correlation analysis as it could reveal

Table S1: Comparison of $P_{int}$ of the elements with the atomic $P_{max}$ of the corresponding hydrides and fluorides with the respective valence.

| **Number** | **Element** | **Valence** | $\mathbf{P_{int}}$**(Element)** | $\mathbf{P_{int}}$**(Hydride)** $[\mathrm{kcal}^{0.5}\,\mathrm{mol}^{-0.5}]$ | $\mathbf{P_{int}}$**(Fluoride)** |
|---|---|---|---|---|---|
| 1 | H | 1 | 6.2 | 6.5 | 6.4 |
| 2 | He | 0 | 4.0 | 4.0 | 4.0 |
| 3 | Li | 1 | 38.0 | 139.8 | 168.2 |
| 4 | Be | 2 | 15.0 | 12.0 | 17.2 |
| 5 | B | 3 | 11.8 | 18.5 | 15.1 |
| 6 | C | 4 | 9.5 | 7.6 | 6.4 |
| 7 | N | 3 | 7.8 | 9.3 | 7.6 |
| 8 | O | 2 | 7.0 | 8.6 | 8.1 |
| 9 | F | 1 | 6.3 | 7.5 | 8.2 |
| 10 | Ne | 0 | 5.7 | 5.7 | 5.7 |
| 11 | Na | 1 | 49.6 | 63.1 | 106.0 |
| 12 | Mg | 2 | 22.0 | 23.5 | 59.0 |
| 13 | Al | 3 | 20.2 | 32.5 | 44.6 |
| 14 | Si | 4 | 15.6 | 17.2 | 21.9 |
| 15 | P | 3 | 12.9 | 16.0 | 16.9 |
| 16 | S | 2 | 12.0 | 16.2 | 16.6 |
| 17 | Cl | 1 | 10.9 | 15.1 | 17.5 |
| 18 | Ar | 0 | 10.2 | 10.2 | 10.2 |
| 19 | K | 1 | 89.3 | 44.0 | 72.6 |
| 20 | Ca | 2 | 31.8 | 56.5 | 102.2 |
| 31 | Ga | 3 | 22.2 | 39.9 | 39.7 |
| 32 | Ge | 4 | 17.6 | 19.4 | 25.1 |
| 33 | As | 3 | 14.8 | 19.5 | 21.7 |
| 34 | Se | 2 | 14.5 | 20.3 | 23.2 |
| 35 | Br | 1 | 13.4 | 19.2 | 23.3 |
| 36 | Kr | 0 | 12.8 | 12.8 | 12.8 |
| 37 | Rb | 1 | 103.8 | 46.4 | 68.7 |
| 38 | Sr | 2 | 39.1 | 53.4 | 88.5 |
| 49 | In | 3 | 25.1 | 35.3 | 41.6 |
| 50 | Sn | 4 | 20.8 | 23.7 | 32.1 |
| 51 | Sb | 3 | 18.0 | 23.3 | 25.4 |
| 52 | Te | 2 | 17.4 | 24.3 | 27.5 |
| 53 | I | 1 | 16.2 | 23.5 | 27.9 |
| 54 | Xe | 0 | 15.6 | 15.6 | 15.6 |
| 55 | Cs | 1 | 126.6 | 43.4 | 64.2 |
| 56 | Ba | 2 | 47.9 | 55.1 | 85.5 |
| 81 | Tl | 3 | 29.5 | 37.8 | 42.1 |
| 82 | Pb | 4 | 24.2 | 27.1 | 38.8 |
| 83 | Bi | 3 | 20.7 | 27.5 | 32.8 |
| 84 | Po | 2 | 19.5 | 29.9 | 38.2 |
| 85 | At | 1 | 18.3 | 29.0 | 36.2 |
| 86 | Rn | 0 | 17.4 | 17.4 | 17.4 |

spurious correlations.

Table S2: Calculated $P_{int}$, $P_{max}$, $V_{rel}$ (relative to Me) and the product of $P_{int}$ and $A_{rel}$ (relative to Me) of common substituents in organic chemistry.

| **Group** | $\mathbf{P_{int}}$ | $\mathbf{P_{max}}$ | $\mathbf{P_{int}}$ $\mathbf{A_{rel}}$ | $\mathbf{V_{rel}}$ |
|---|---|---|---|---|
| | | [kcal$^{0.5}$ mol$^{-0.5}$] | | |
| -H | 3.6 | 6.2 | 1.5 | 0.29 |
| -F | 6.1 | 7.0 | 3.5 | 0.43 |
| -OH | 7.8 | 10.1 | 5.5 | 0.62 |
| -$NH_2$ | 8.7 | 12.0 | 7.4 | 0.81 |
| -CN | 9.6 | 11.0 | 10.0 | 1.03 |
| -Me | 9.8 | 12.5 | 9.8 | 1.00 |
| -NC | 10.1 | 12.2 | 10.9 | 1.07 |
| -$CF_3$ | 10.3 | 16.5 | 14.1 | 1.48 |
| -$NO_2$ | 10.4 | 15.2 | 12.5 | 1.24 |
| -OMe | 10.4 | 14.8 | 13.4 | 1.36 |
| -COOH | 10.9 | 15.4 | 14.4 | 1.41 |
| -CCH | 10.9 | 11.8 | 13.0 | 1.24 |
| -$B(OH)_2$ | 10.9 | 15.6 | 16.1 | 1.62 |
| -$CONH_2$ | 11.3 | 15.9 | 16.3 | 1.60 |
| -Cl | 11.4 | 14.9 | 10.6 | 0.93 |
| -Et | 11.5 | 16.0 | 17.5 | 1.72 |
| -Ac | 11.6 | 17.2 | 18.4 | 1.80 |
| -$CHCH_2$ | 11.6 | 16.5 | 15.7 | 1.49 |
| -$CF_2CF_3$ | 11.9 | 19.0 | 24.5 | 2.49 |
| -*i*Pr | 12.3 | 18.7 | 24.4 | 2.43 |
| -SH | 12.3 | 17.4 | 13.5 | 1.18 |
| -*c*Pr | 12.4 | 19.5 | 21.7 | 2.07 |
| -OCOMe | 12.6 | 18.5 | 23.4 | 2.13 |
| -COOMe | 12.6 | 19.9 | 23.3 | 2.12 |
| -*t*Bu | 12.9 | 18.4 | 30.6 | 3.13 |
| -$CF(CF_3)_2$ | 13.0 | 23.3 | 34.2 | 3.45 |
| -Br | 13.5 | 19.5 | 15.0 | 1.20 |
| -$CONMe_2$ | 13.5 | 21.8 | 31.7 | 2.95 |
| -$C(CF_3)_3$ | 13.9 | 21.3 | 43.0 | 4.35 |
| -$SO_3H$ | 14.6 | 23.3 | 25.1 | 2.01 |
| -SeH | 14.6 | 22.2 | 18.3 | 1.39 |
| -TMS | 14.7 | 23.4 | 42.6 | 3.71 |
| Cy | 14.7 | 20.4 | 42.5 | 4.01 |
| -$OPO_3H_2$ | 15.1 | 26.1 | 31.6 | 2.51 |
| -Ph | 15.3 | 23.3 | 38.6 | 3.30 |
| -OTf | 15.3 | 26.0 | 38.6 | 3.19 |
| -TIPS | 16.3 | 26.8 | 79.7 | 7.78 |
| -I | 16.3 | 25.1 | 22.0 | 1.57 |
| -TPS | 19.2 | 36.4 | 132.9 | 10.49 |

Table S3: Comparison of calculated $P_{int}$ of common substituents in organic chemistry using either PBE (PBE) or promolecular (Pro) densities and either D4 or D3 dispersion corrections. "n.d." means not determined because the densities were not available.

| **Group** | $P_{int}$ [$kcal^{0.5}\,mol^{-0.5}$] | | | |
|---|---|---|---|---|
| | **PBE, D4** | **PBE, D3** | **Pro, D4** | **Pro, D3** |
| -H | 3.6 | 4.5 | 3.2 | 4.0 |
| -F | 6.1 | 5.1 | 7.1 | 5.9 |
| -OH | 7.8 | 8.0 | 7.7 | 7.7 |
| -$NH_2$ | 8.7 | 9.3 | 8.4 | 8.9 |
| -CN | 9.6 | 9.4 | 12.2 | 11.9 |
| -Me | 9.8 | 10.3 | 8.7 | 9.2 |
| -NC | 10.1 | 10.2 | 12.6 | 12.8 |
| -$CF_3$ | 10.3 | 8.8 | 12.4 | 10.5 |
| -$NO_2$ | 10.4 | 8.8 | 13.3 | 11.2 |
| -OMe | 10.4 | 10.4 | 10.4 | 10.2 |
| -COOH | 10.9 | 10.4 | 12.3 | 11.5 |
| -CCH | 10.9 | 10.9 | 11.9 | 11.9 |
| -$B(OH)_2$ | 10.9 | 11.5 | 11.2 | 11.4 |
| -$CONH_2$ | 11.3 | 11.2 | 12.2 | 11.9 |
| -Cl | 11.4 | 10.8 | 14.1 | 13.3 |
| -Et | 11.5 | 11.8 | 10.6 | 10.9 |
| -Ac | 11.6 | 11.5 | 12.0 | 11.8 |
| -$CHCH_2$ | 11.6 | 11.7 | 11.3 | 11.5 |
| -$CF_2CF_3$ | 11.9 | 10.3 | 14.1 | 12.2 |
| -*i*Pr | 12.3 | 12.5 | 11.7 | 11.9 |
| -SH | 12.3 | 12.1 | 14.3 | 14.0 |
| -*c*Pr | 12.4 | 12.5 | 11.6 | 11.8 |
| -OCOMe | 12.6 | 12.2 | 12.9 | 12.5 |
| -COOMe | 12.6 | 12.2 | 13.1 | 12.6 |
| -*t*Bu | 12.9 | 13.1 | 12.4 | 12.6 |
| -$CF(CF_3)_2$ | 13.0 | 11.3 | 15.3 | 13.2 |
| -Br | 13.5 | 12.8 | 17.6 | 16.8 |
| -$CONMe_2$ | 13.5 | 13.4 | 13.5 | 13.3 |
| -$C(CF_3)_3$ | 13.9 | 12.1 | 16.2 | 14.0 |
| -$SO_3H$ | 14.6 | 13.3 | 16.8 | 15.0 |
| -SeH | 14.6 | 14.2 | 17.5 | 17.0 |
| -TMS | 14.7 | 15.1 | 13.7 | 14.1 |
| Cy | 14.7 | 14.8 | 14.0 | 14.1 |
| -$OPO_3H_2$ | 15.1 | 14.6 | 16.4 | 15.4 |
| -Ph | 15.3 | 15.0 | 15.4 | 15.1 |
| -OTf | 15.3 | 13.3 | 18.0 | 15.6 |
| -TIPS | 16.3 | 16.5 | 15.6 | 15.8 |
| -I | 16.3 | 15.9 | n.d. | n.d. |
| -TPS | 19.2 | 18.9 | 19.6 | 19.2 |

### 2.1.2 Dispersion Maps

In the main text, we already showed the benchmark dispersion map of benzene at the SAPT2+(3)δMP2/aTZ level of theory. In this section, we present benchmark dispersion maps for ethane, ethene, ethyne, perfluoroethane, benzene, pyrrole, furan, thiophene, selenophene, tellurophene, a copper(I) N-heterocyclic carbene complex and a palladium(II) diimine complex. We benchmarked the LDP maps against the dispersion energies between the molecules and noble gas atoms placed at the molecular surface. To compute dispersion, we used D3,[4] D4,[5,6] dDsC,[52–54] VV10,[47,48] XDM,[57–61] several SAPT[33] methods and LED.[39] For the DFT dispersion corrections employed, we used the optimized damping parameters of B3LYP. The corresponding results are shown in Figures S1-S99. For every benchmark dispersion map, the corresponding interacting noble gas atom is explicitly stated. Notably, qualitatively wrong results are obtained for the LDP maps of ethyne. However, as all the values on the surface of ethyne are very similar and in a very narrow range, small differences will have a significant effect. We attribute the systematic problem of the LDP maps from D3 or D4 at least partially to the improper account of many-body dispersion. Furthermore, the copper(I) N-heterocyclic carbene and the palladium(II) diimine complex also show some systematic differences but the position of the local extrema are well reproduced in the LDP maps.

**Ethane**

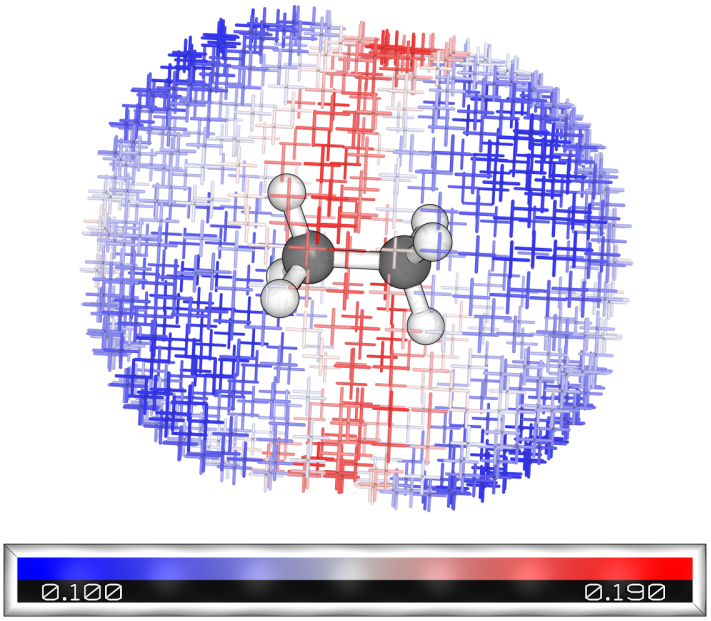



Figure S1: Benchmark dispersion map from D3 with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

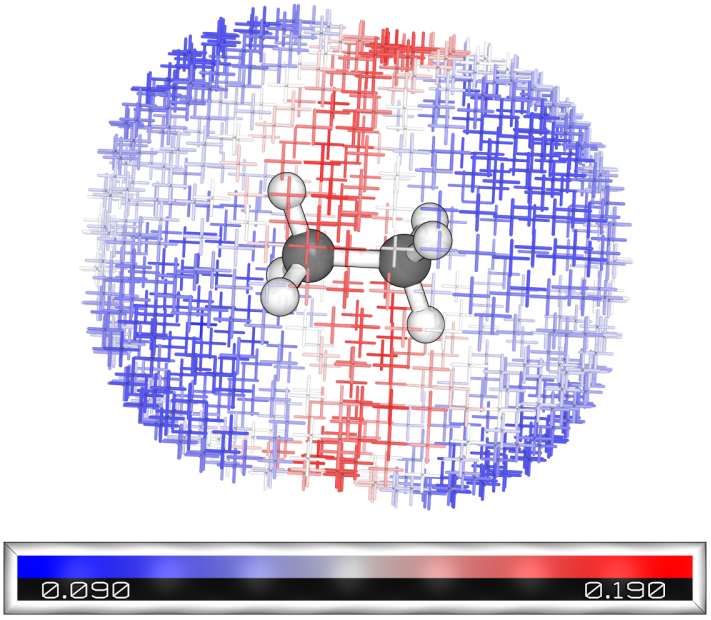



Figure S2: Benchmark dispersion map from D4 with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

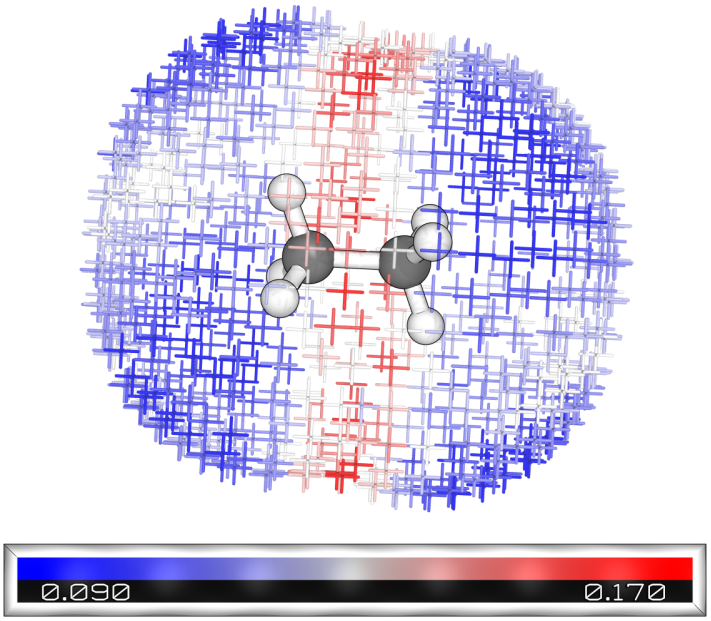



Figure S3: Benchmark dispersion map from LED with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

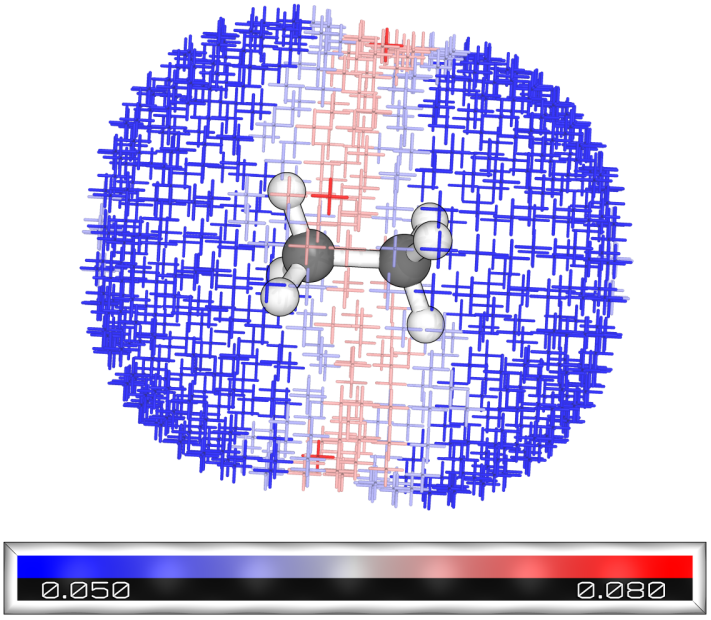



Figure S4: Benchmark dispersion map from sSAPT0 with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

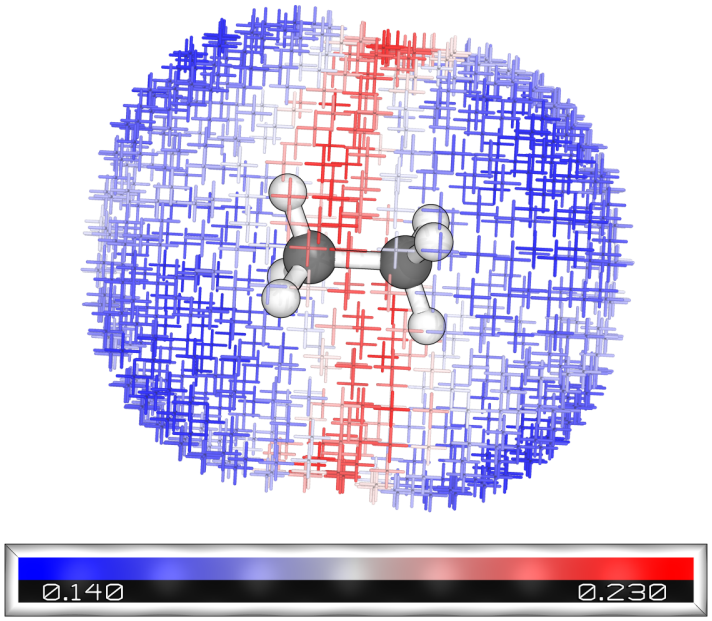



Figure S5: Benchmark dispersion map from SAPT2+ with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

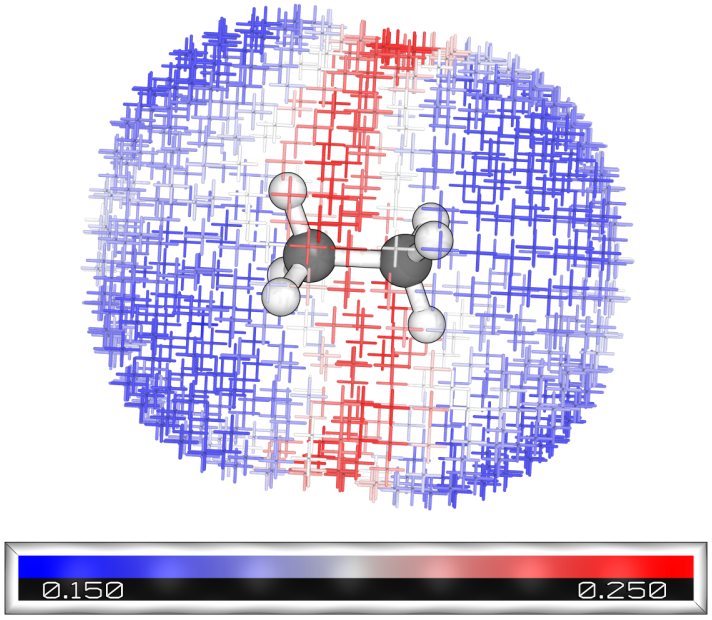



Figure S6: Benchmark dispersion map from SAPT2+(3) with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

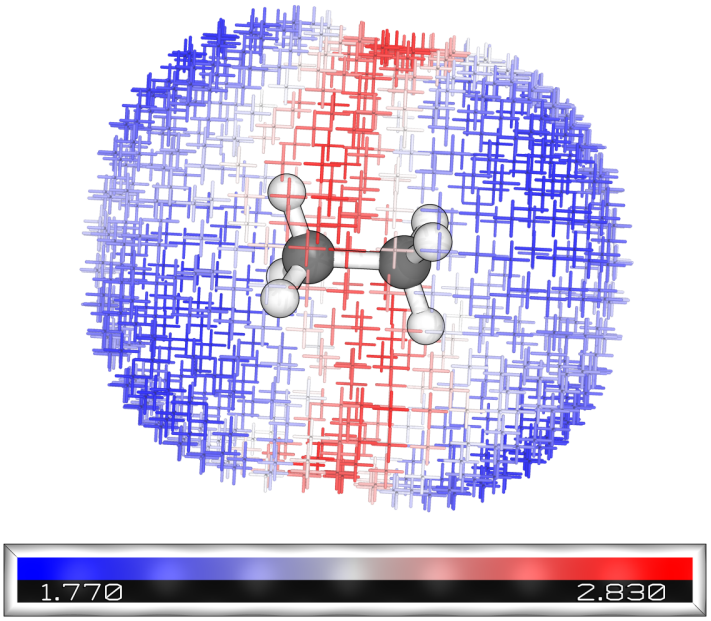



Figure S7: Sparse LDP map with D3 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

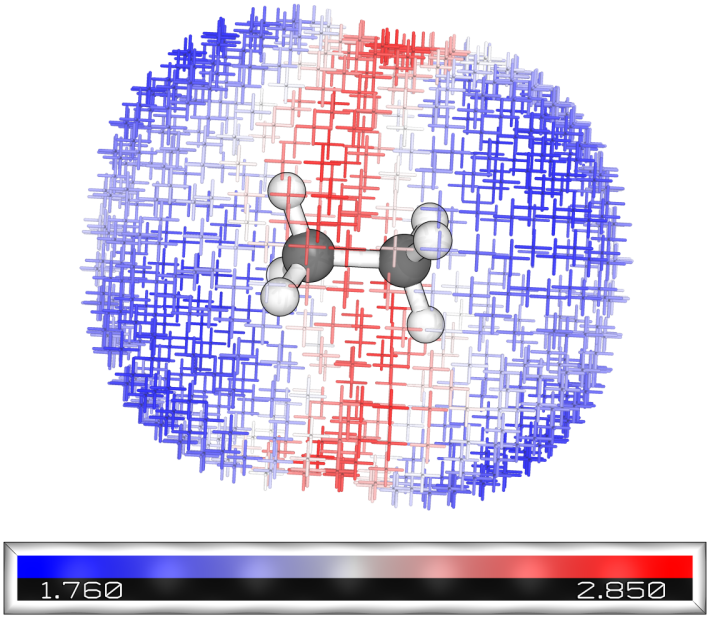



Figure S8: Sparse LDP map with D4 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

**Ethene**

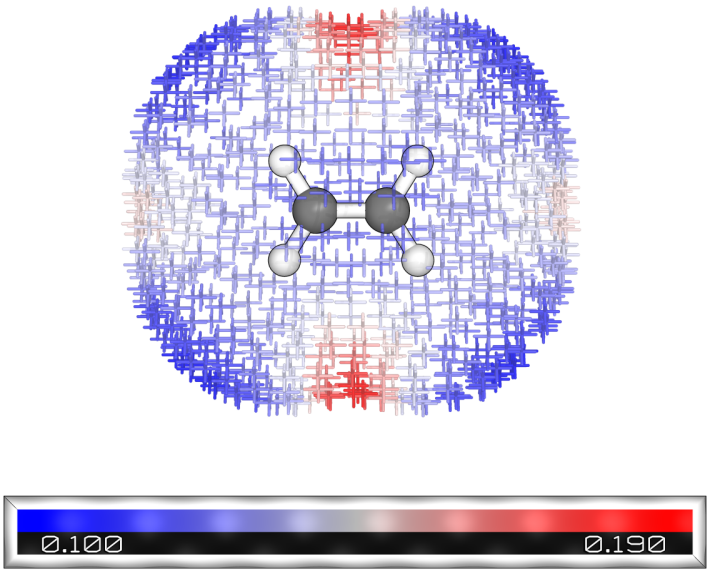



Figure S9: Benchmark dispersion map from D3 with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

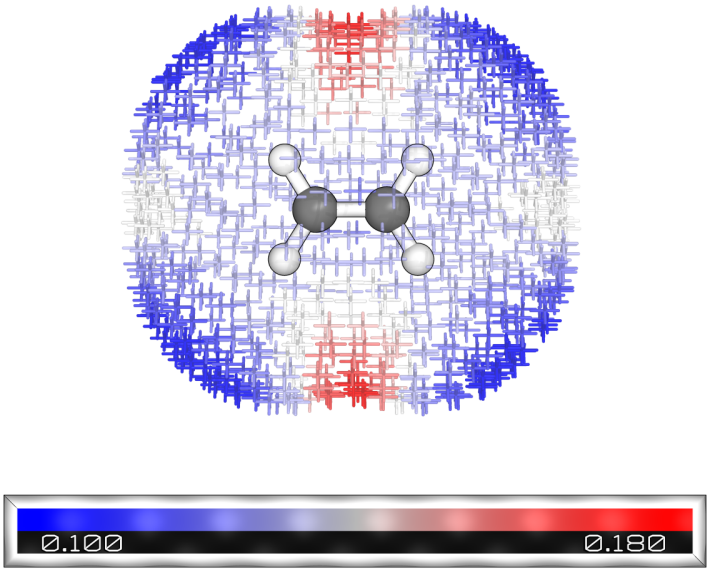



Figure S10: Benchmark dispersion map from D4 with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

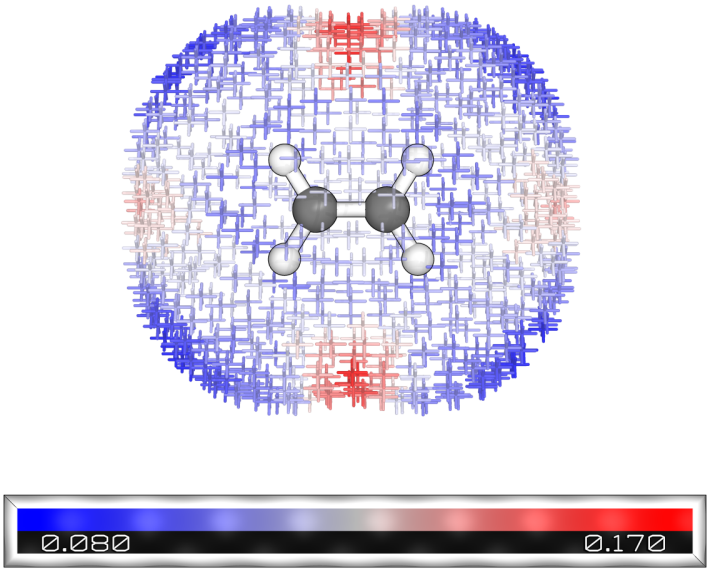



Figure S11: Benchmark dispersion map from LED with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

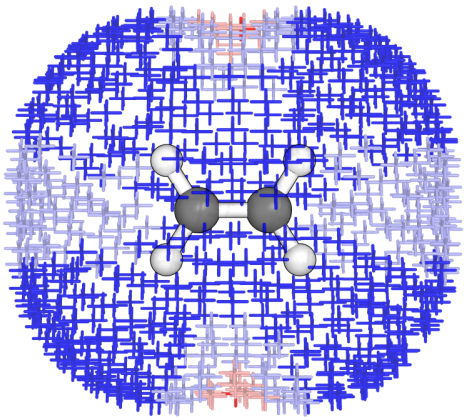


Figure S12: Benchmark dispersion map from sSAPT0 with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

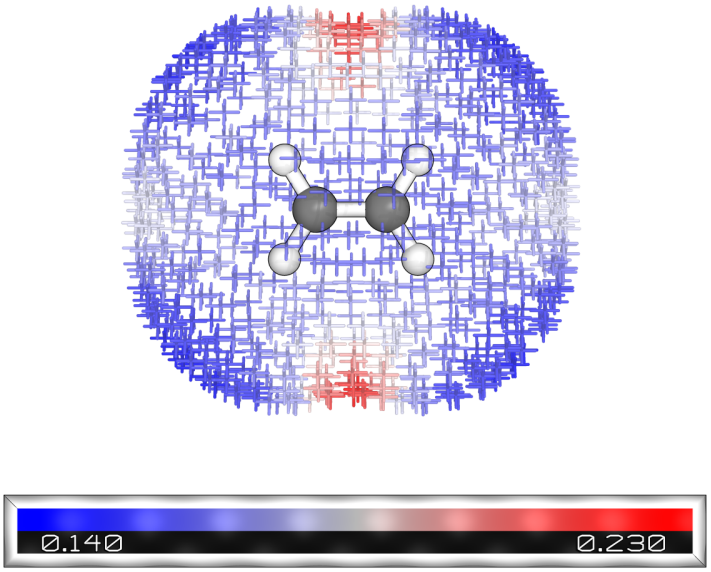



Figure S13: Benchmark dispersion map from SAPT2+ with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

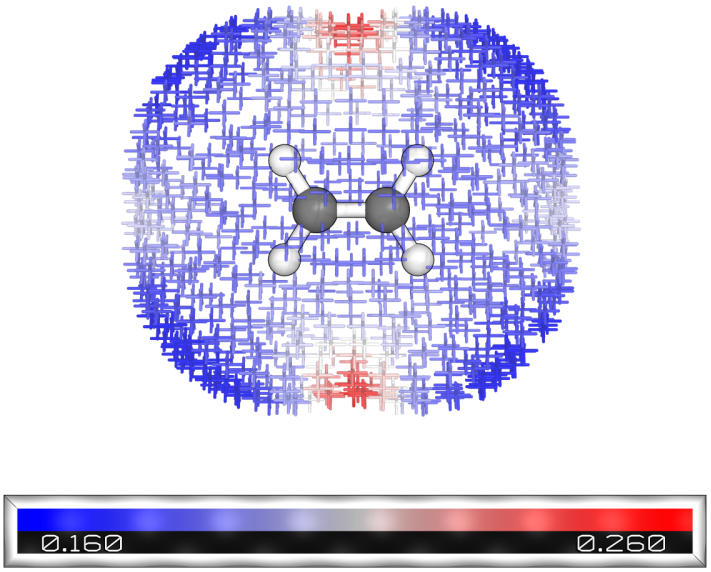



Figure S14: Benchmark dispersion map from SAPT2+(3) with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

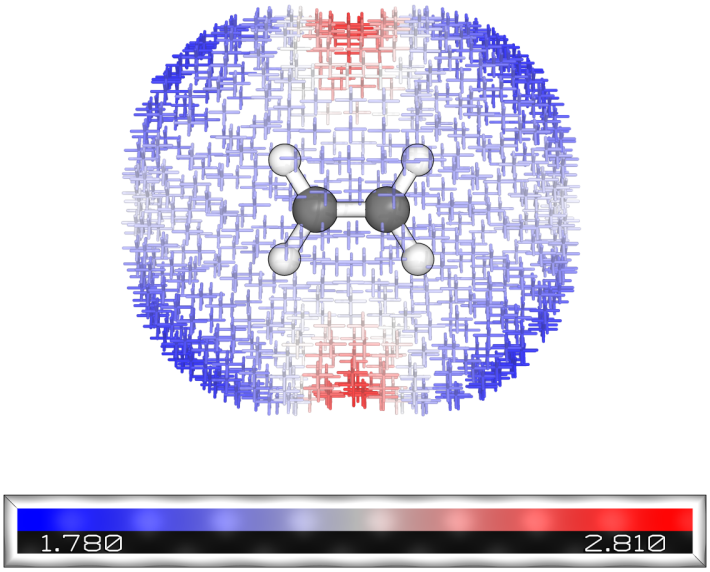



Figure S15: Sparse LDP map with D3 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

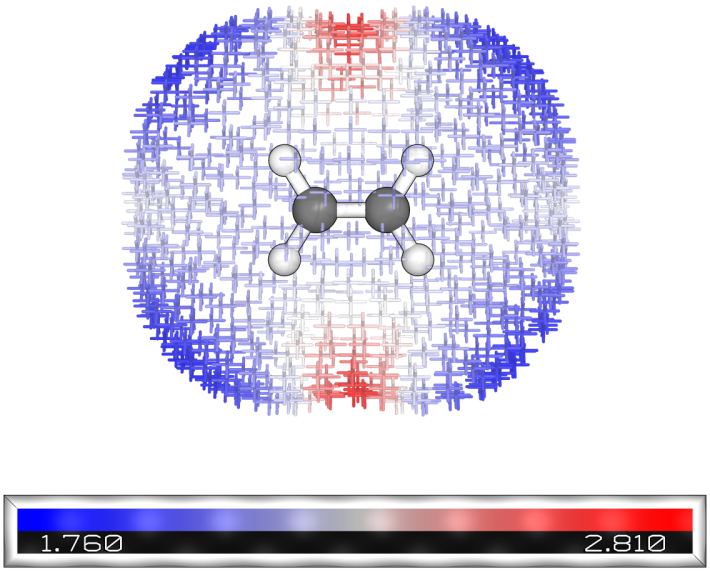



Figure S16: Sparse LDP map with D4 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

**Ethyne**

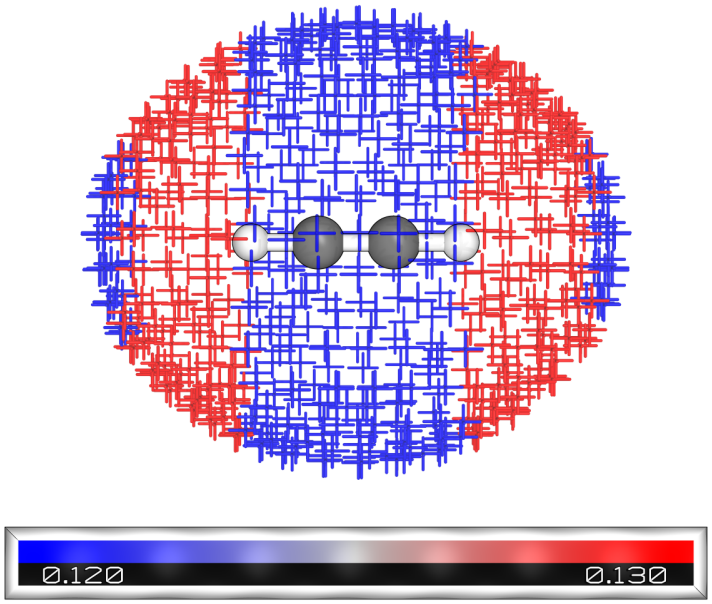



Figure S17: Benchmark dispersion map from D3 with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

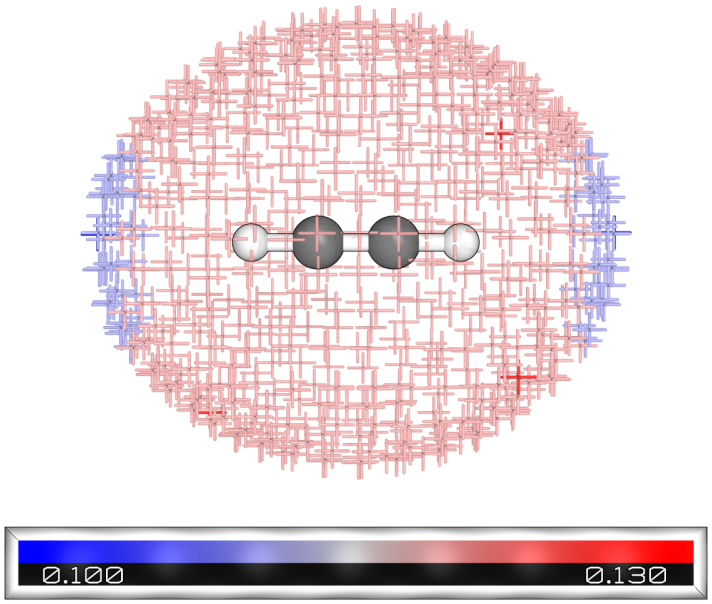



Figure S18: Benchmark dispersion map from D4 with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

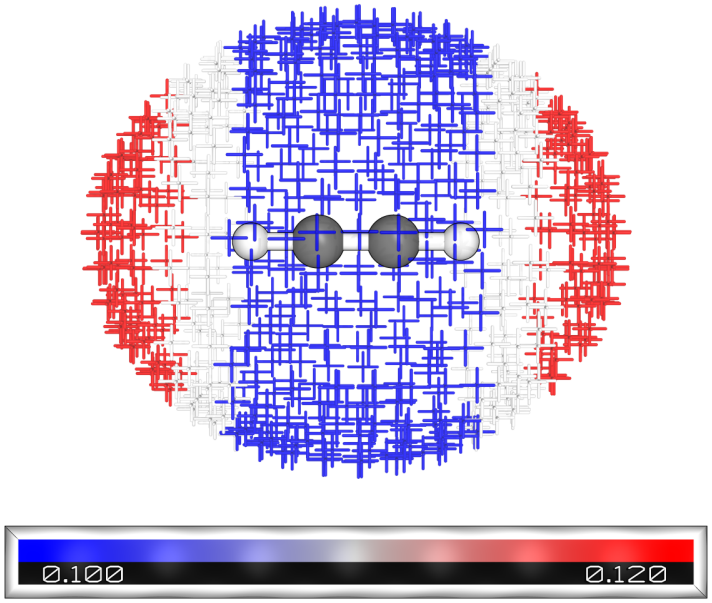



Figure S19: Benchmark dispersion map from LED with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

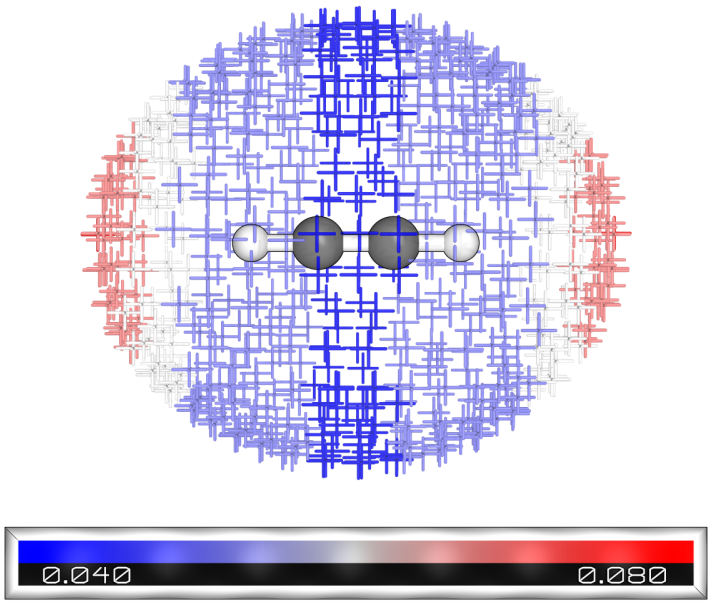



Figure S20: Benchmark dispersion map from sSAPT0 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

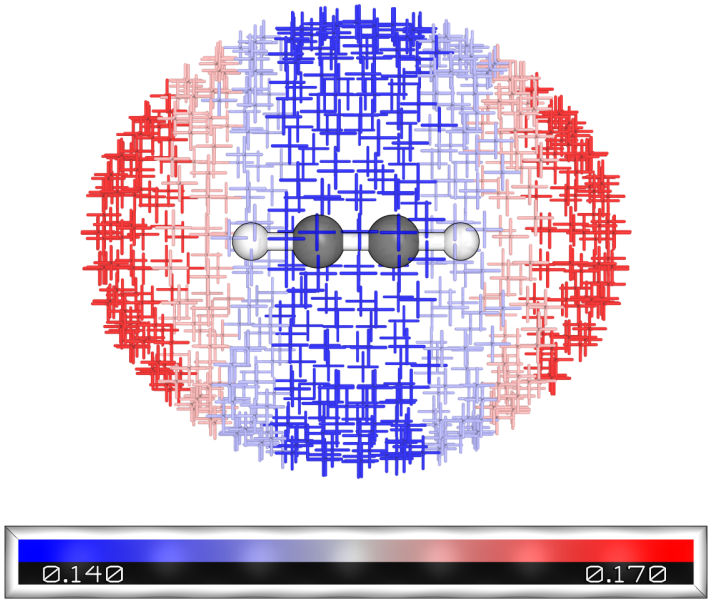



Figure S21: Benchmark dispersion map from SAPT2+ with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

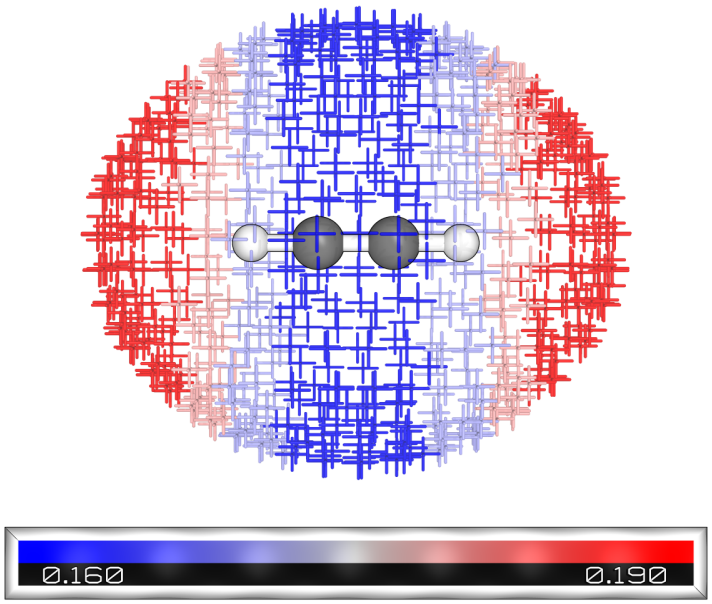



Figure S22: Benchmark dispersion map from SAPT2+(3) with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

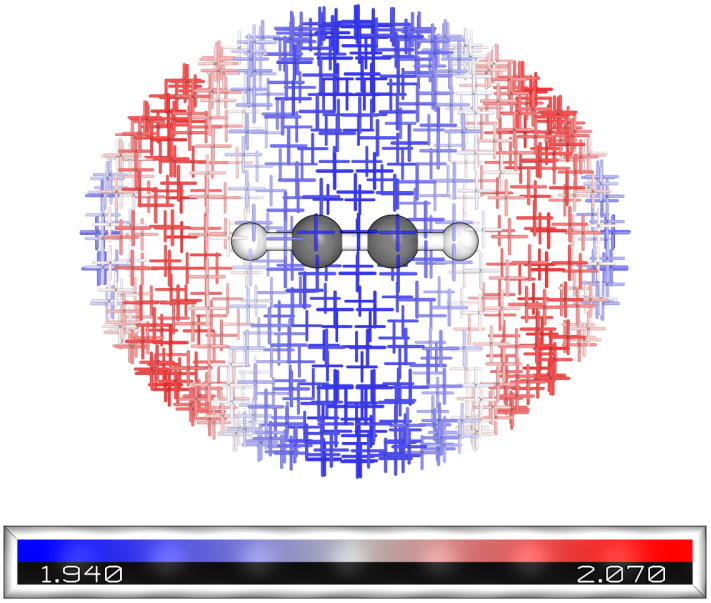



Figure S23: Sparse LDP map with D3 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

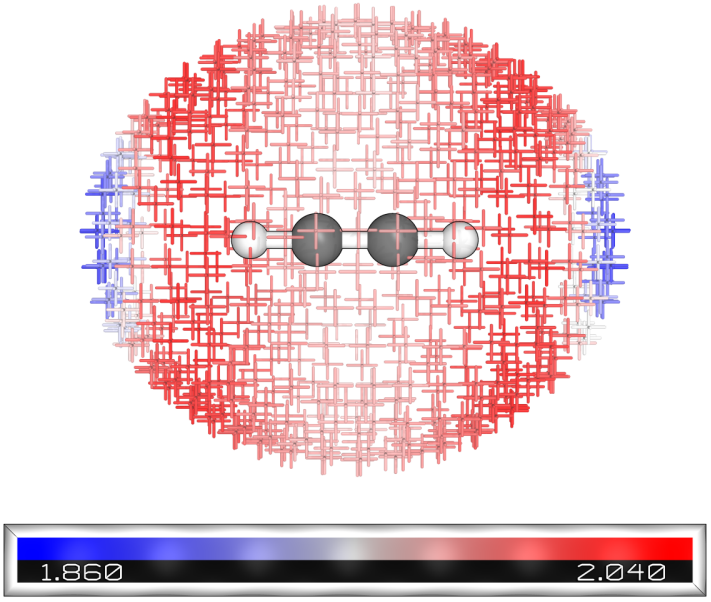



Figure S24: Sparse LDP map with D4 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

**Perfluoroethane**

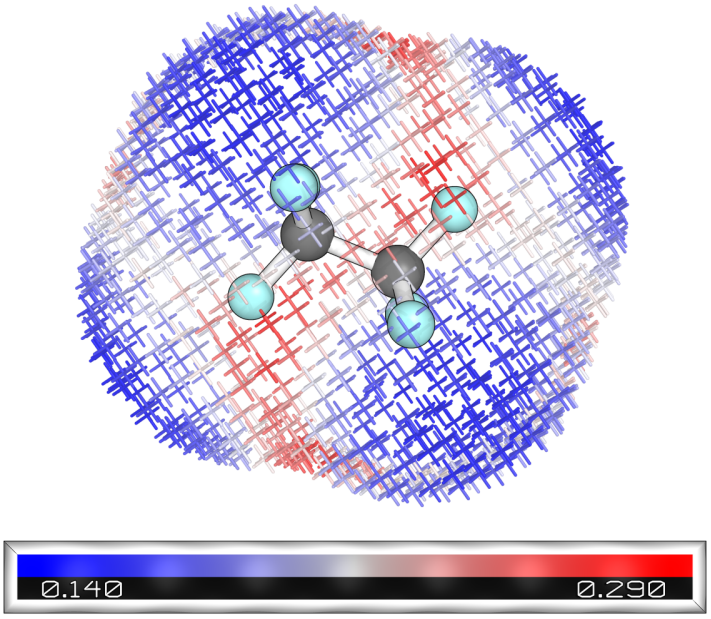



Figure S25: Benchmark dispersion map from D3 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

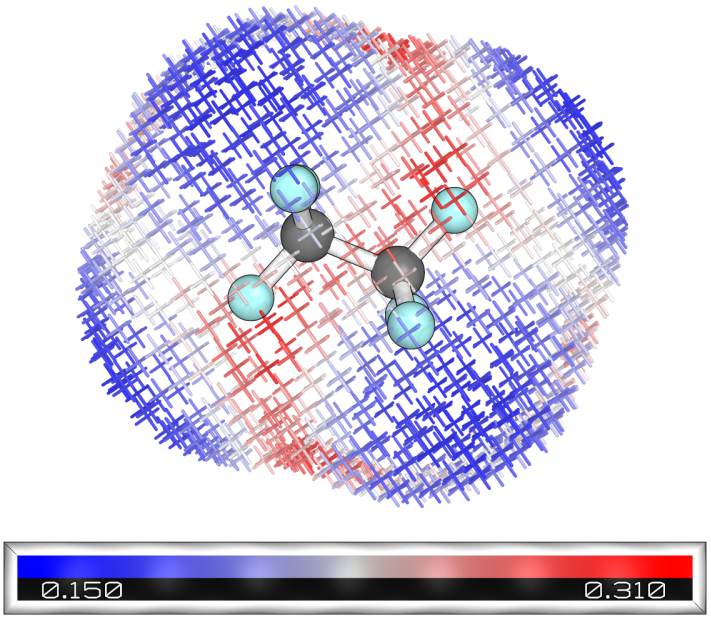



Figure S26: Benchmark dispersion map from D4 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

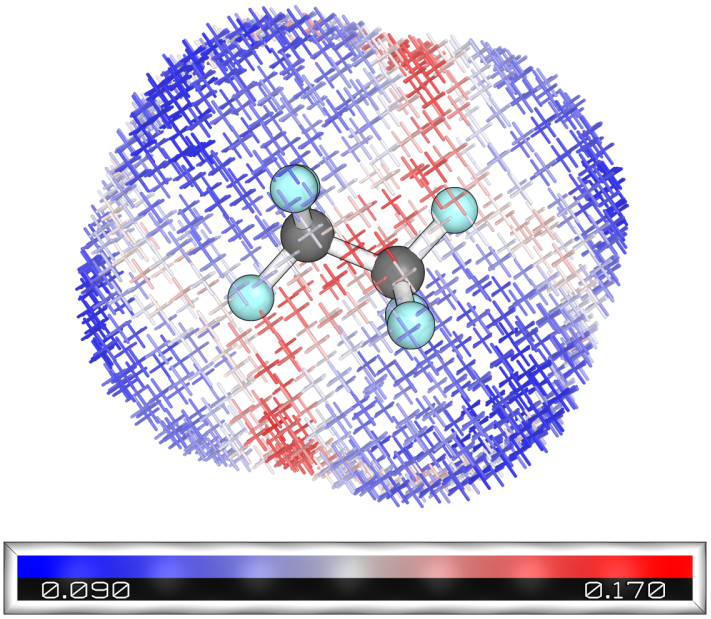



Figure S27: Benchmark dispersion map from LED with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

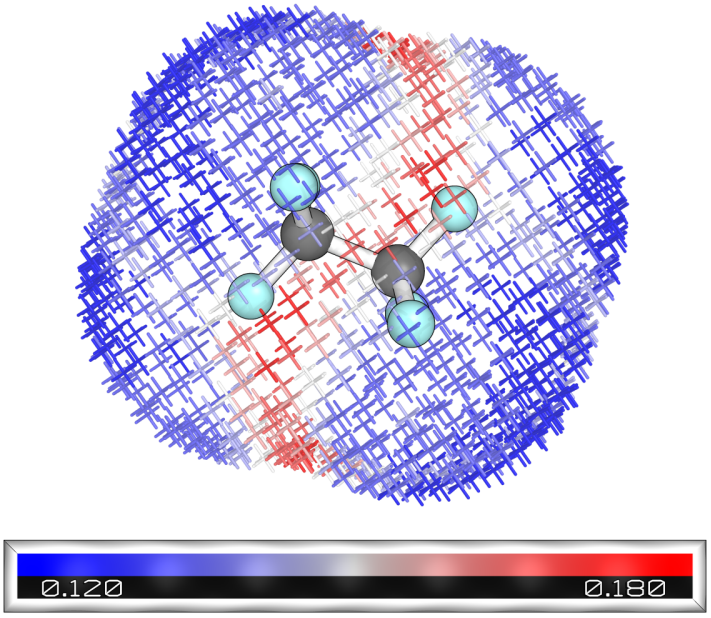



Figure S28: Benchmark dispersion map from sSAPT0 with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

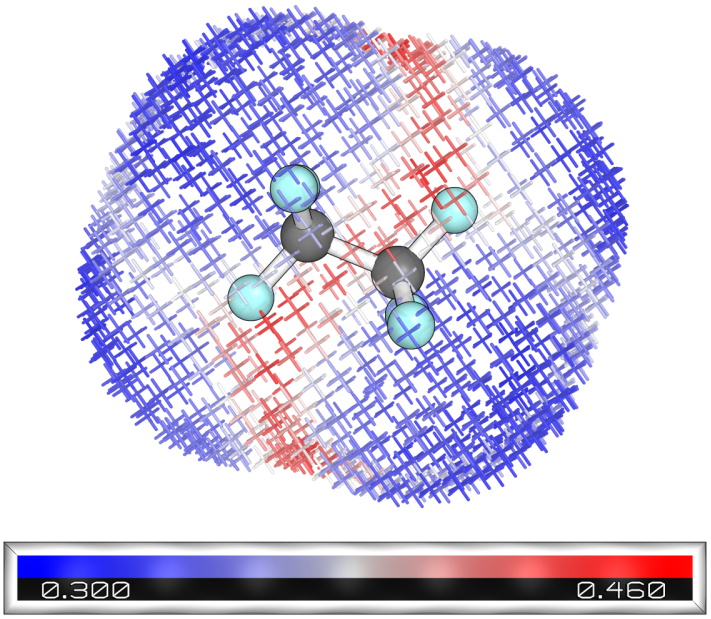



Figure S29: Benchmark dispersion map from SAPT2+ with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

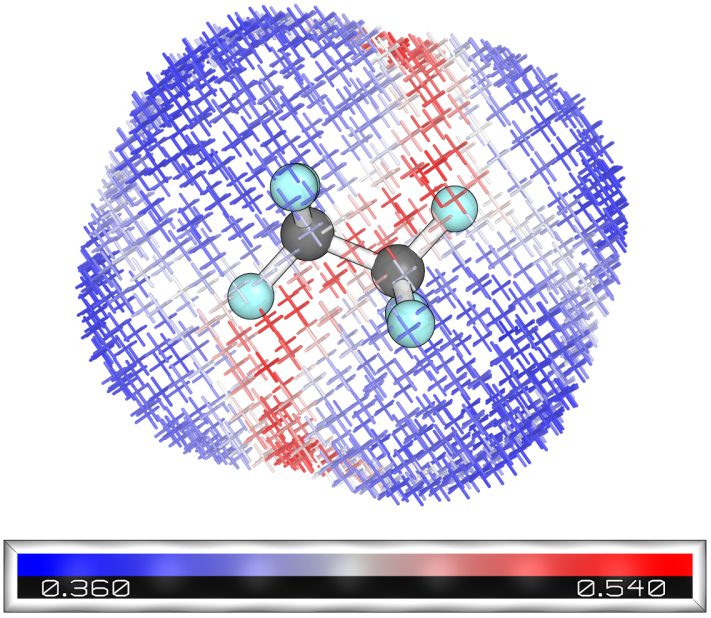



Figure S30: Benchmark dispersion map from SAPT2+(3) with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

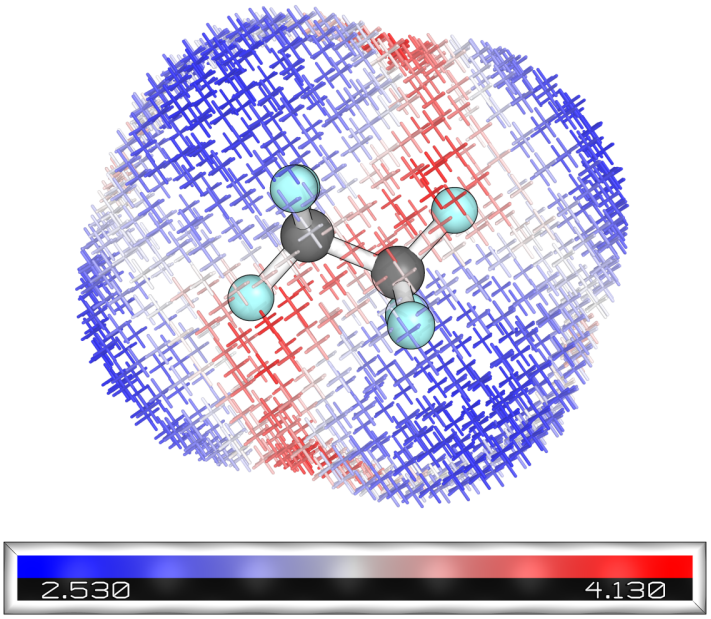



Figure S31: Sparse LDP map with D3 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

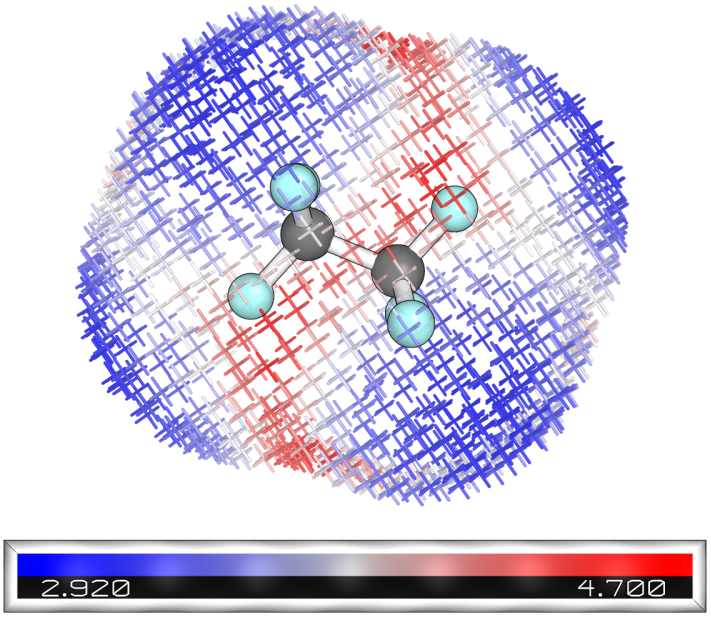



Figure S32: Sparse LDP map with D4 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

**Benzene**

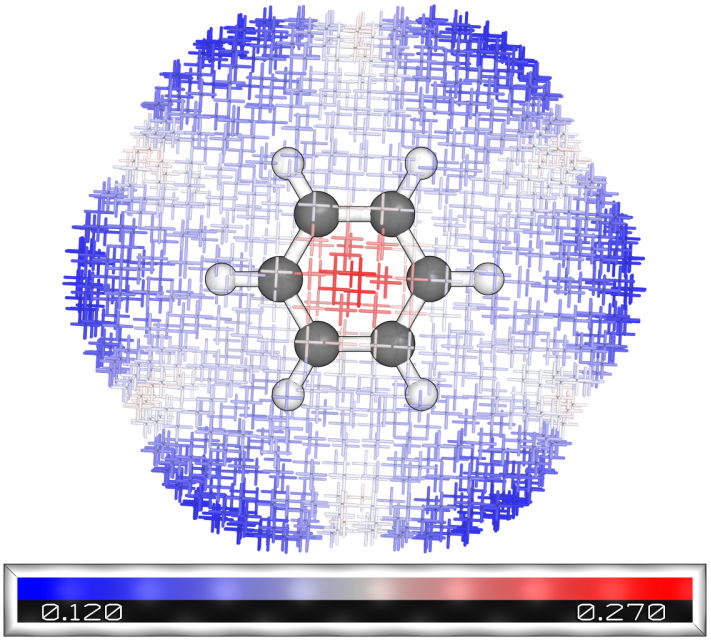



Figure S33: Benchmark dispersion map from D3 with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

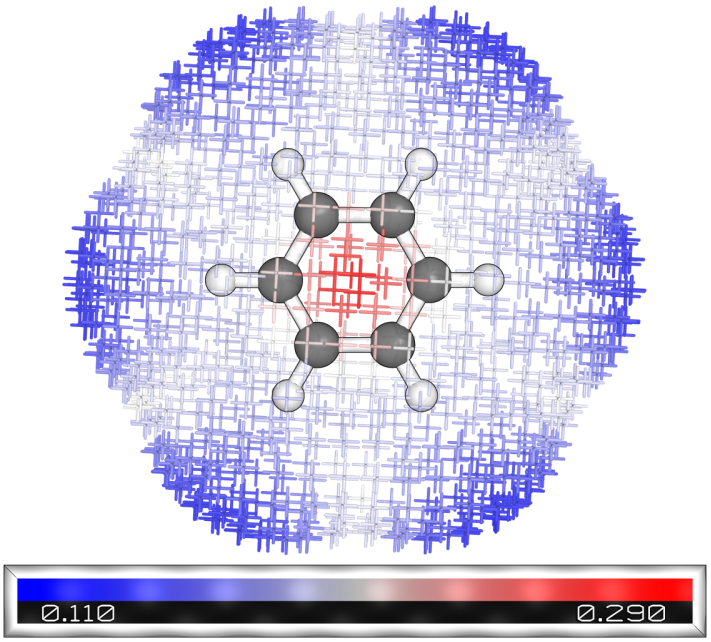



Figure S34: Benchmark dispersion map from D4 with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

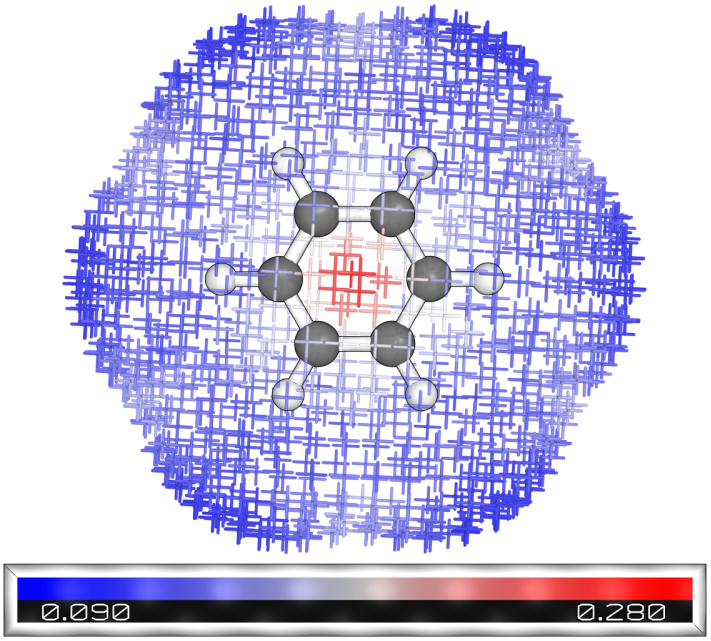



Figure S35: Benchmark dispersion map from LED with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

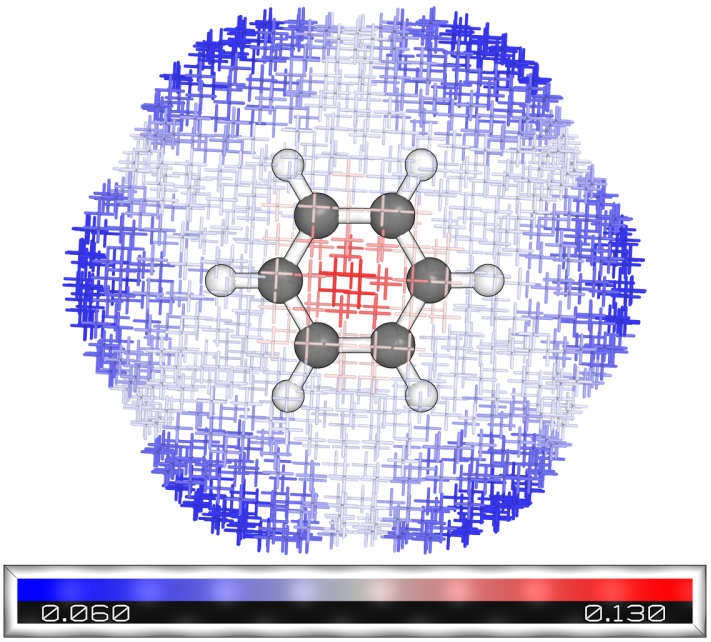



Figure S36: Benchmark dispersion map from sSAPT0 with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

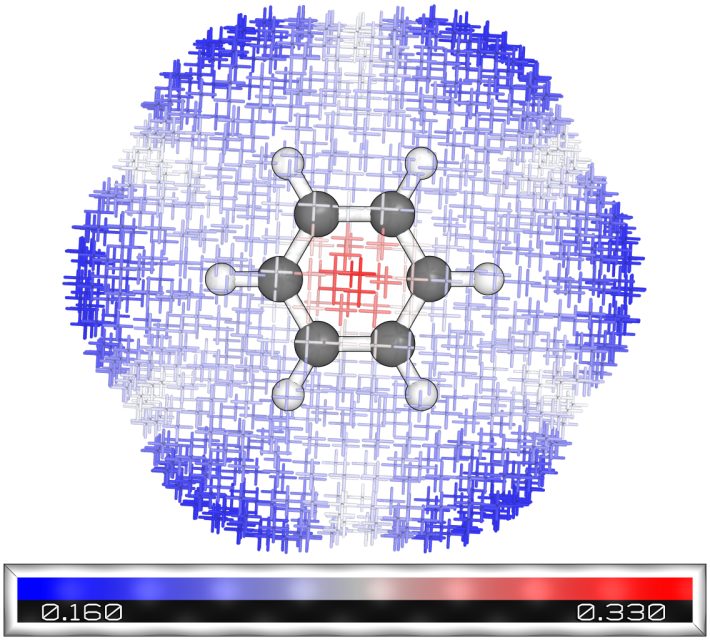



Figure S37: Benchmark dispersion map from SAPT2+ with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

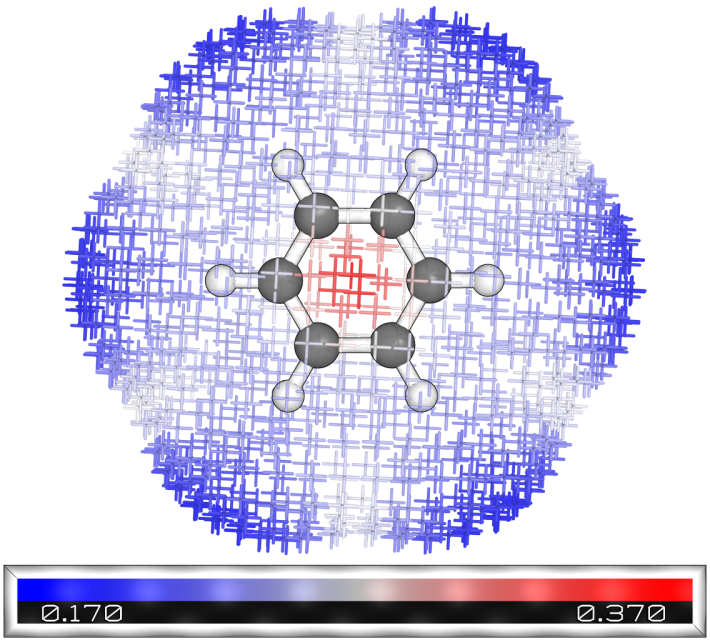



Figure S38: Benchmark dispersion map from SAPT2+(3) with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

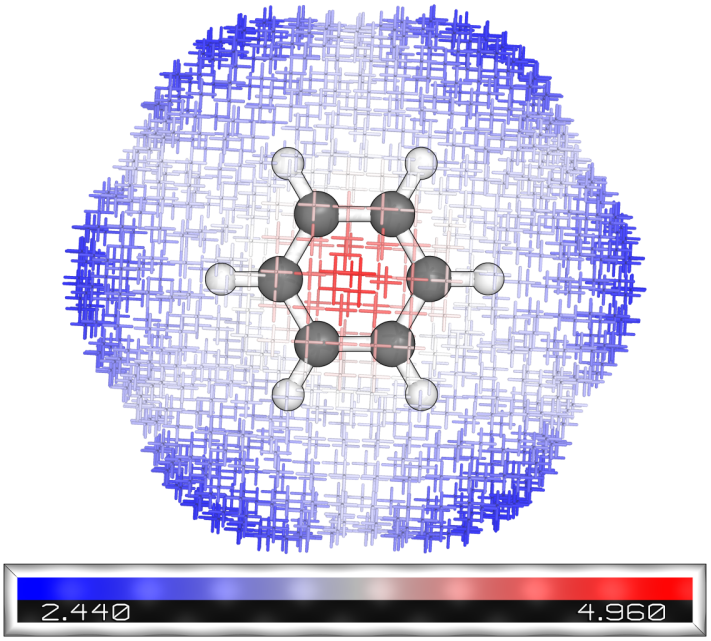



Figure S39: Sparse LDP map with D3 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

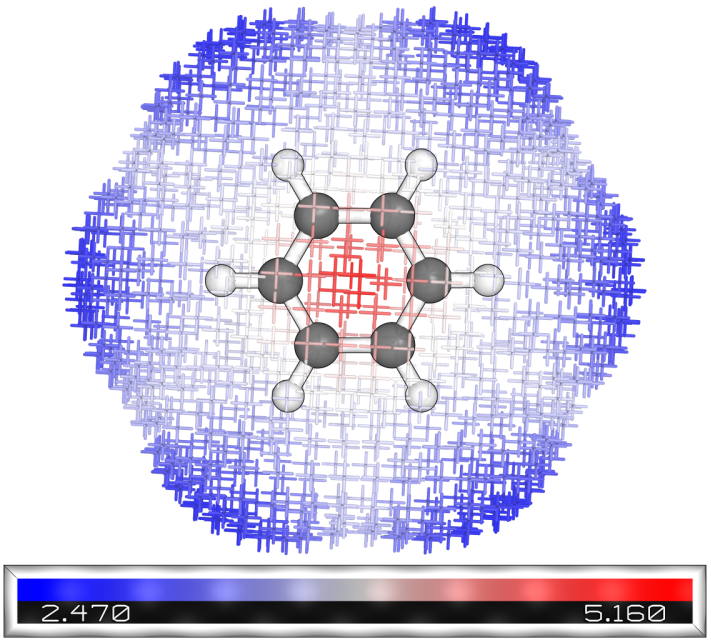



Figure S40: Sparse LDP map with D4 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

**Pyrrole**

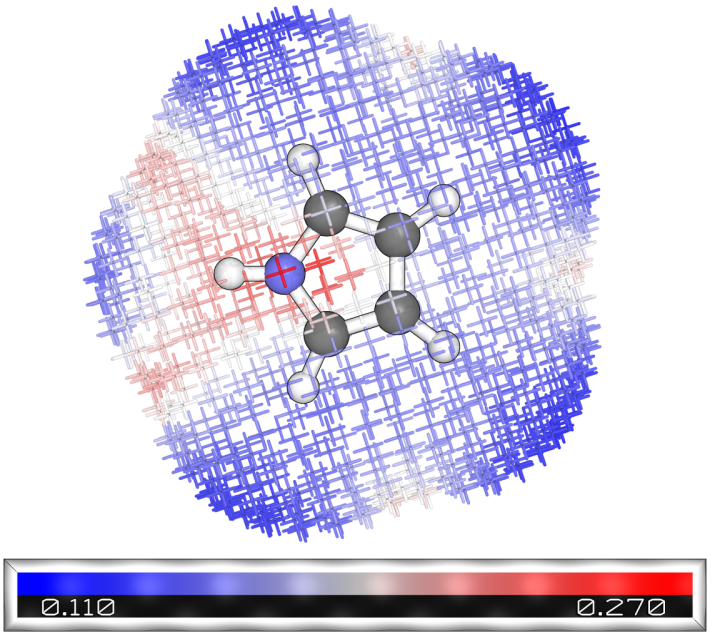



Figure S41: Benchmark dispersion map from D3 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

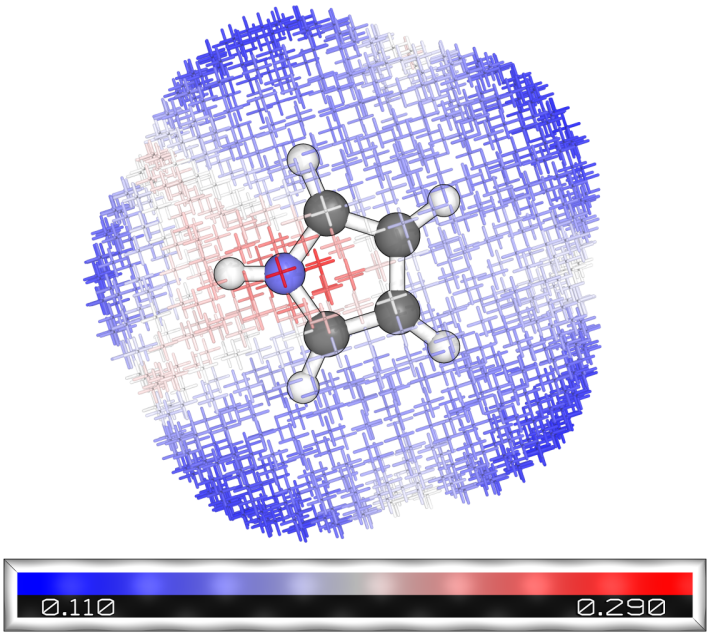



Figure S42: Benchmark dispersion map from D4 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

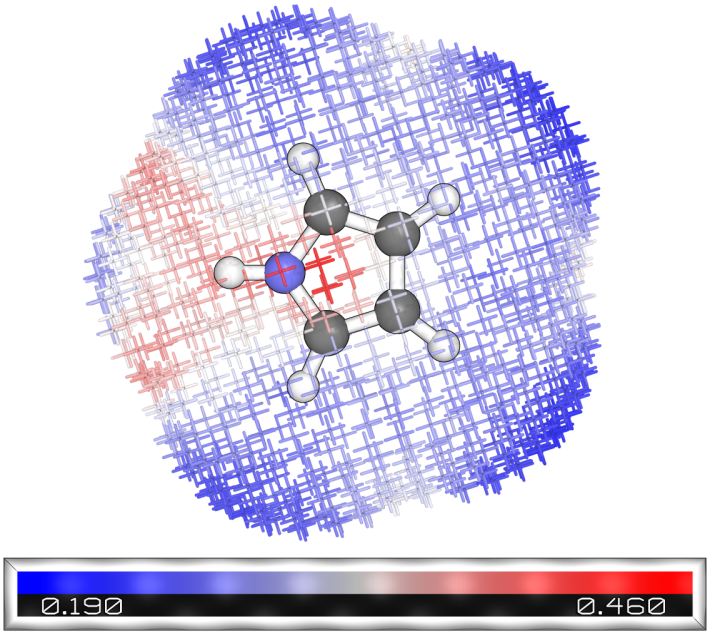



Figure S43: Benchmark dispersion map from LED with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

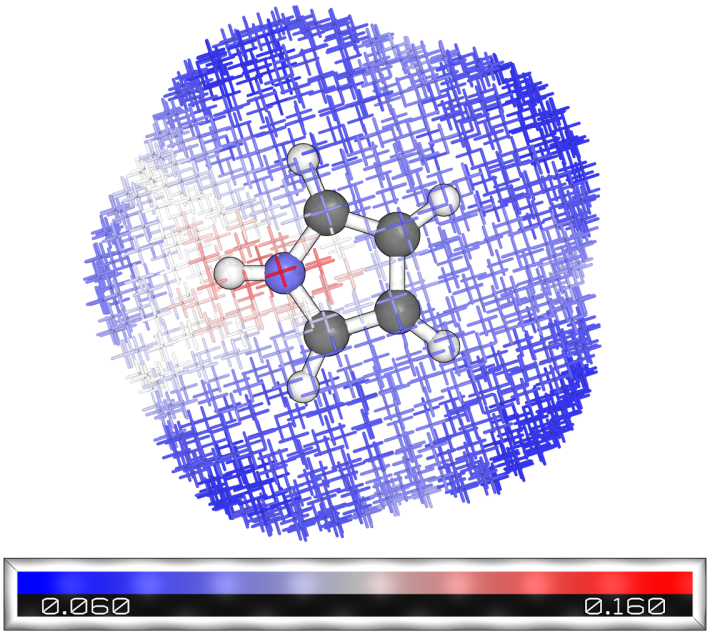



Figure S44: Benchmark dispersion map from sSAPT0 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

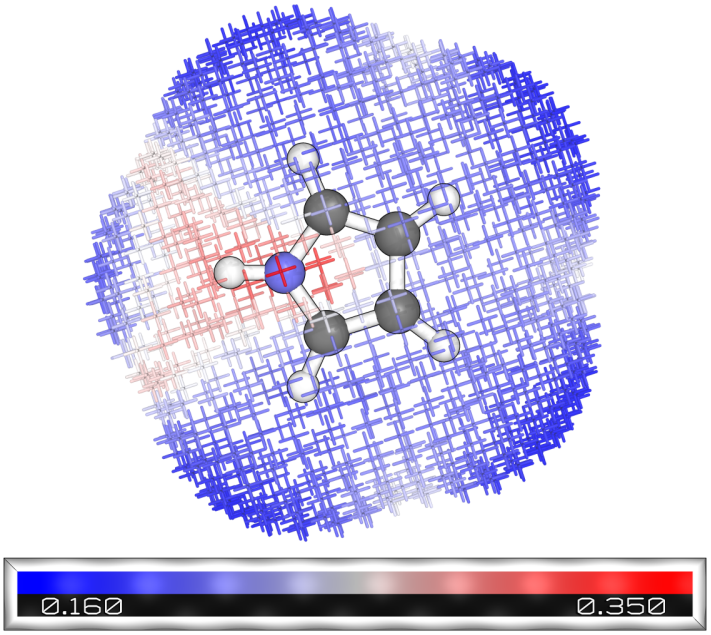



Figure S45: Benchmark dispersion map from SAPT2+ with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

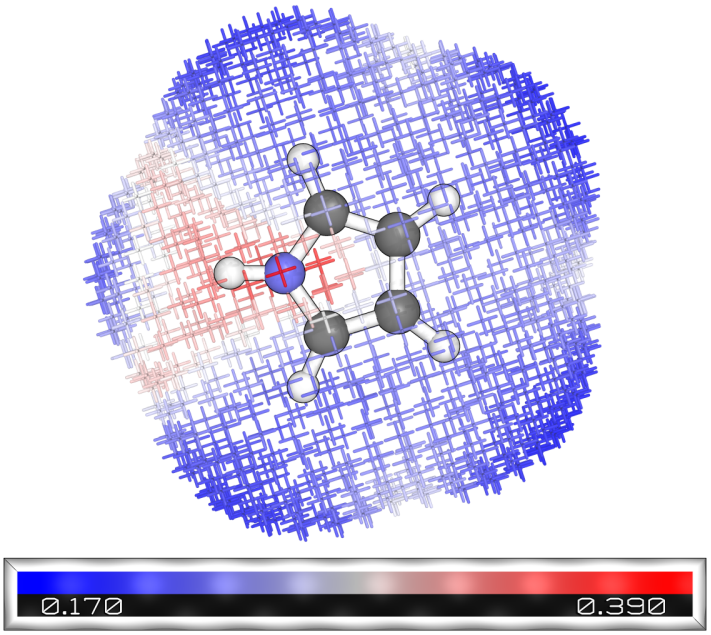



Figure S46: Benchmark dispersion map from SAPT2+(3) with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

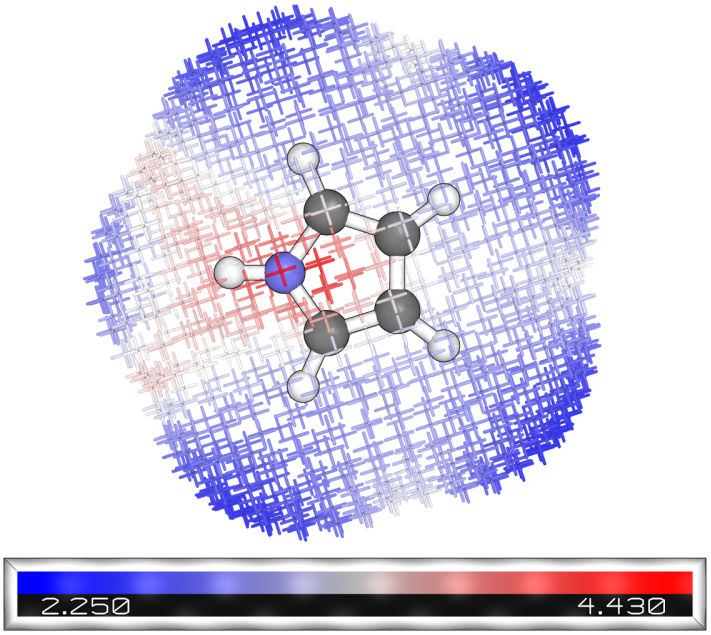



Figure S47: Sparse LDP map with D3 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

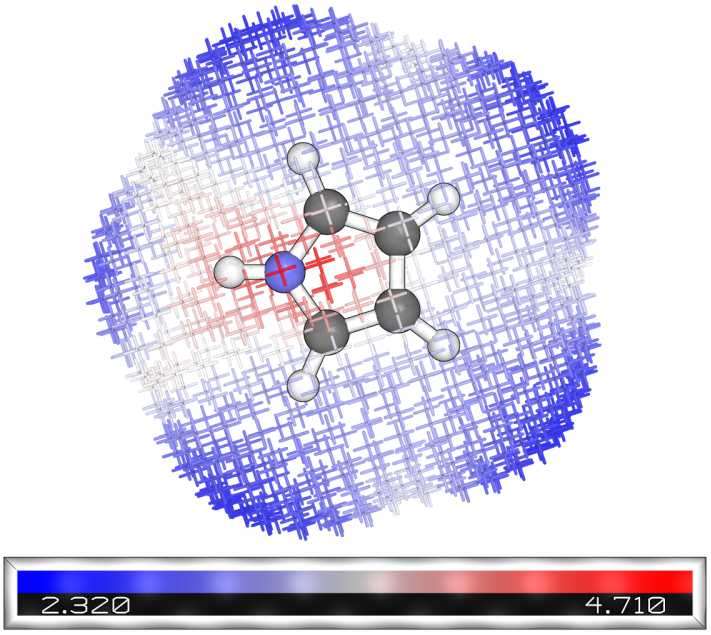



Figure S48: Sparse LDP map with D4 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

**Furan**

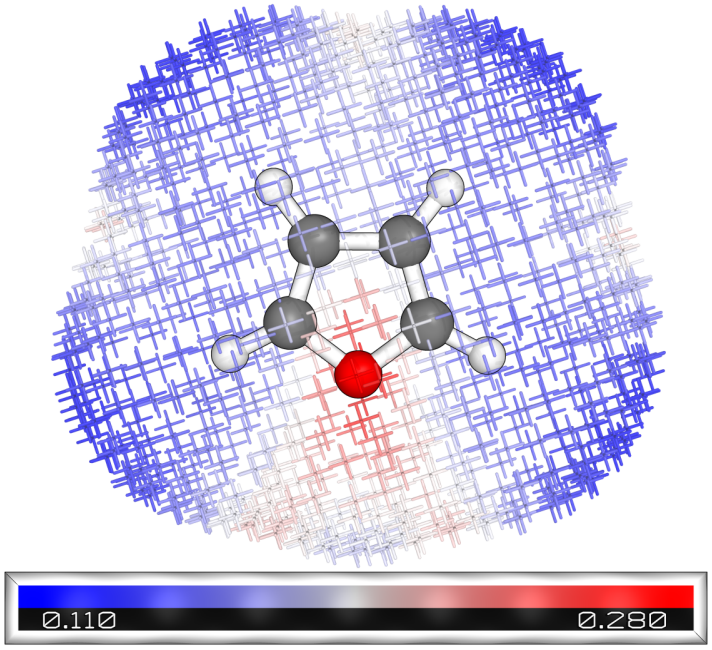



Figure S49: Benchmark dispersion map from D3 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

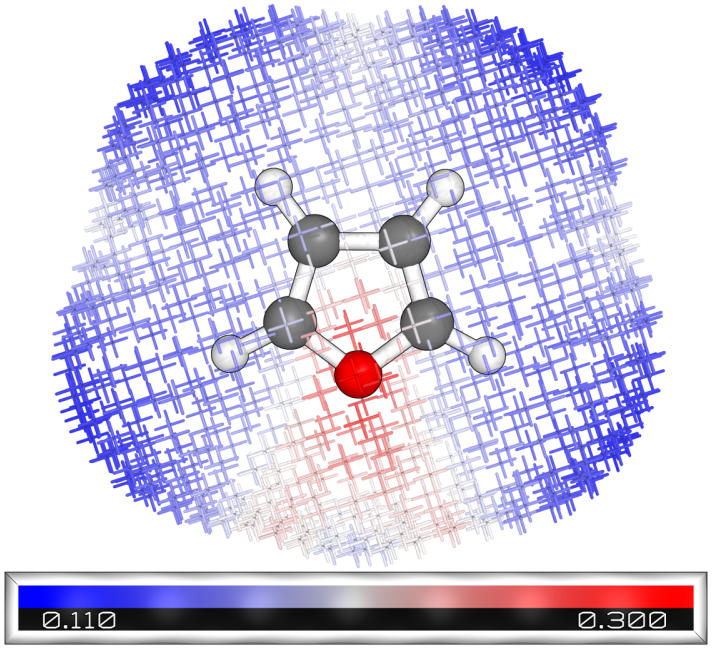



Figure S50: Benchmark dispersion map from D4 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

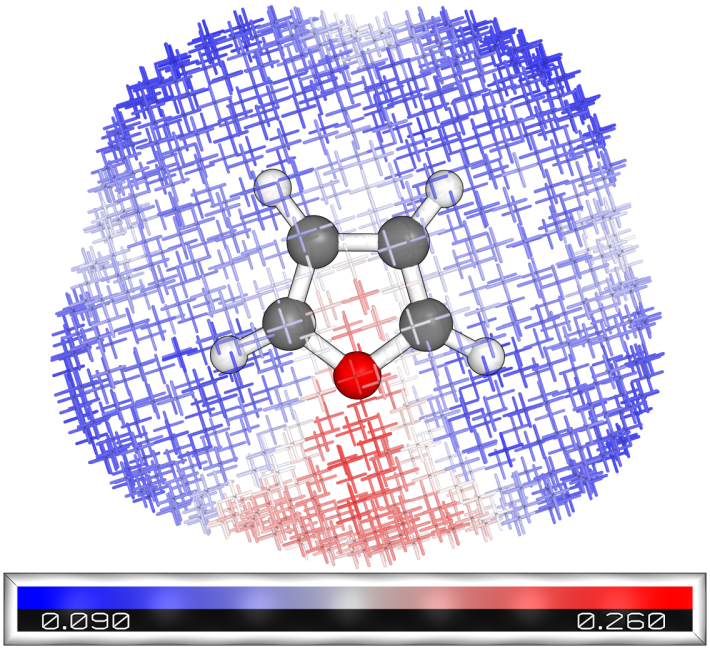



Figure S51: Benchmark dispersion map from LED with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

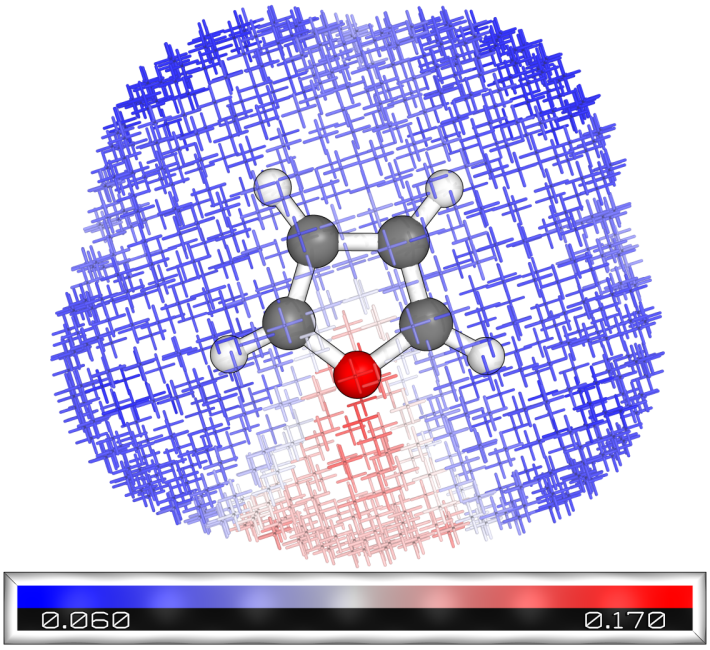



Figure S52: Benchmark dispersion map from sSAPT0 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

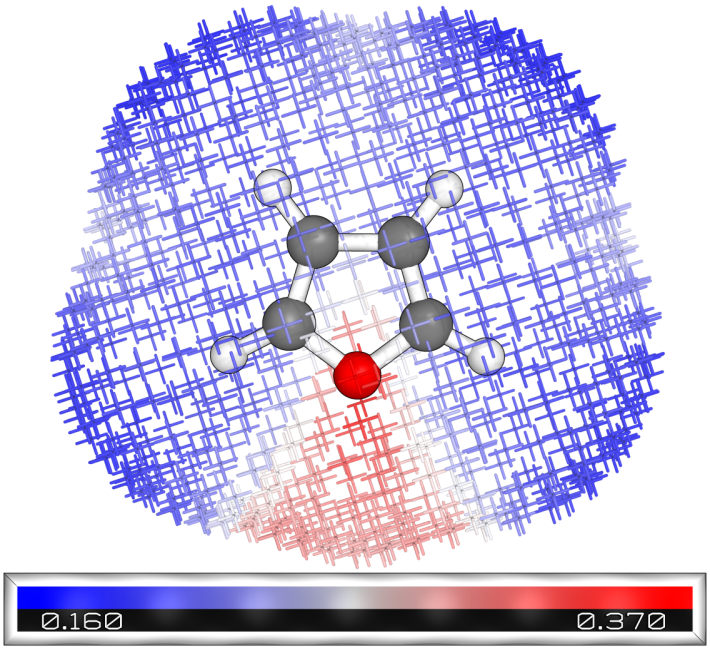



Figure S53: Benchmark dispersion map from SAPT2+ with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

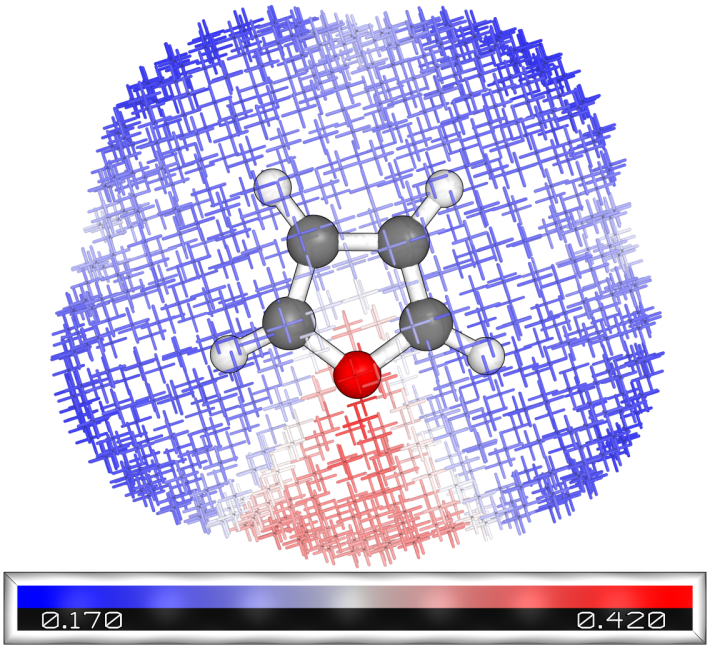



Figure S54: Benchmark dispersion map from SAPT2+(3) with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

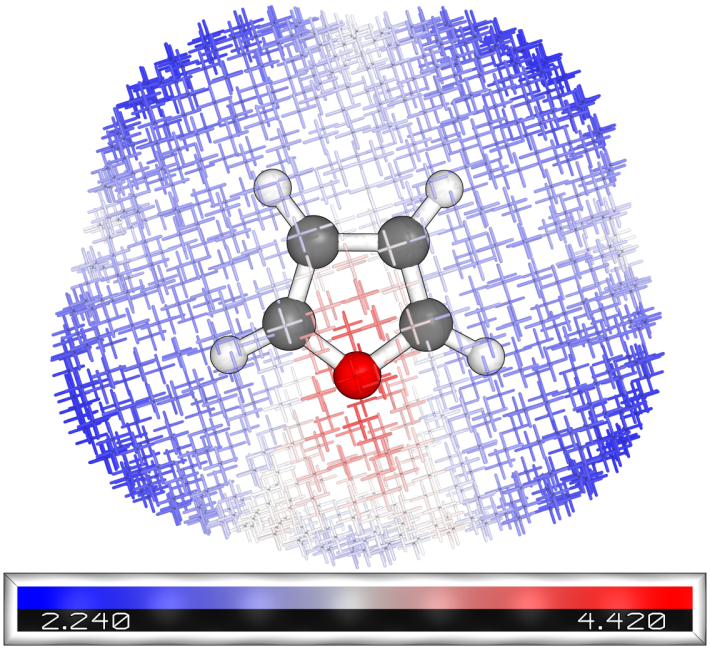



Figure S55: Sparse LDP map with D3 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

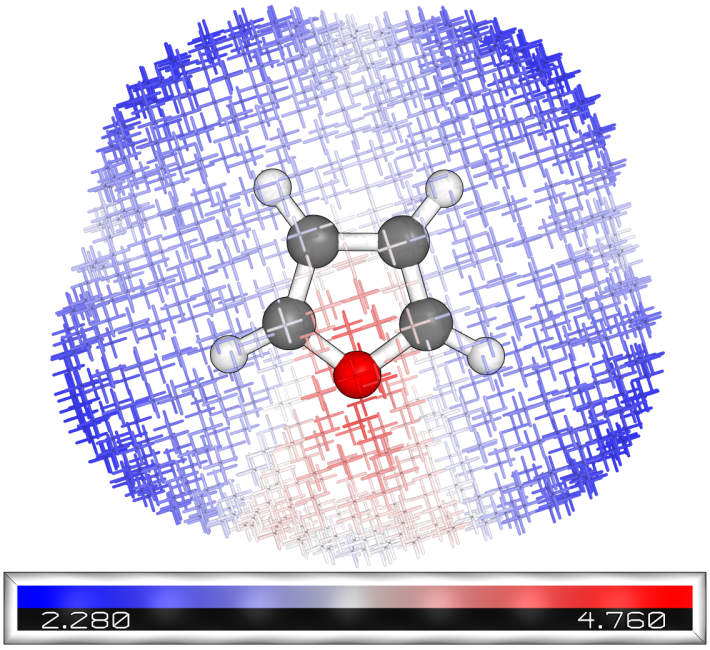



Figure S56: Sparse LDP map with D4 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

**Thiophene**

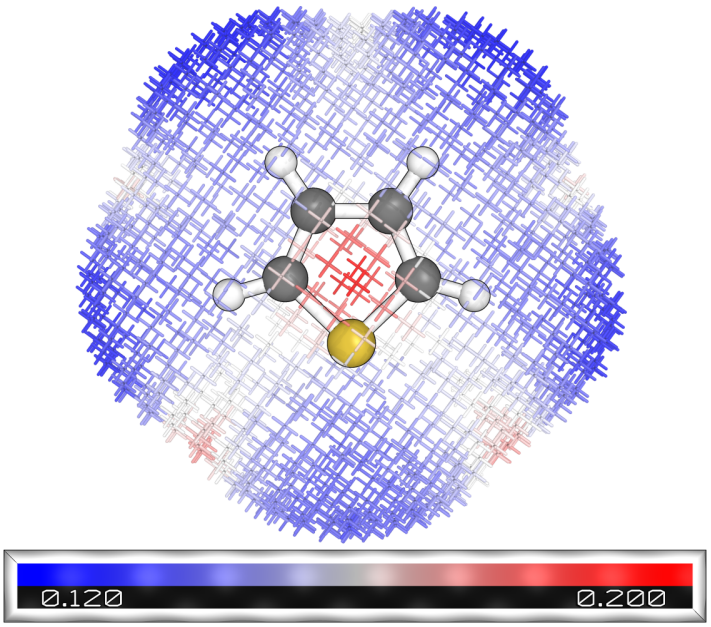



Figure S57: Benchmark dispersion map from D3 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

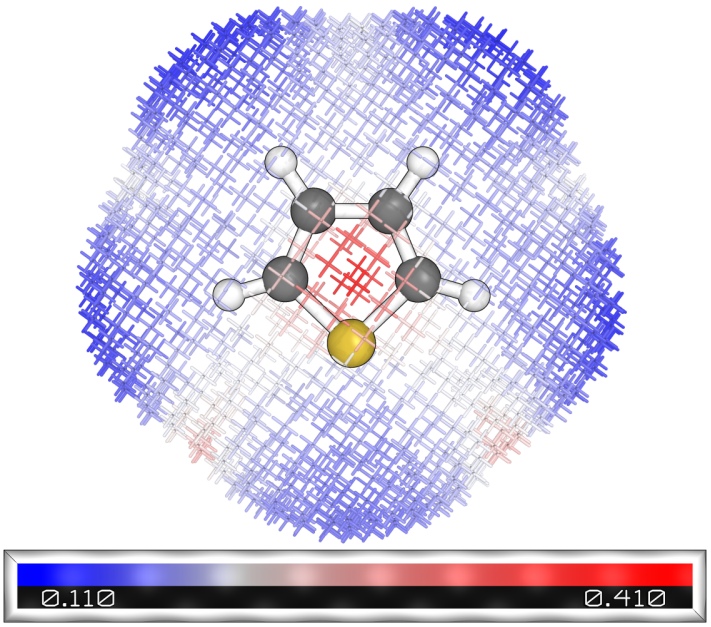



Figure S58: Benchmark dispersion map from D4 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

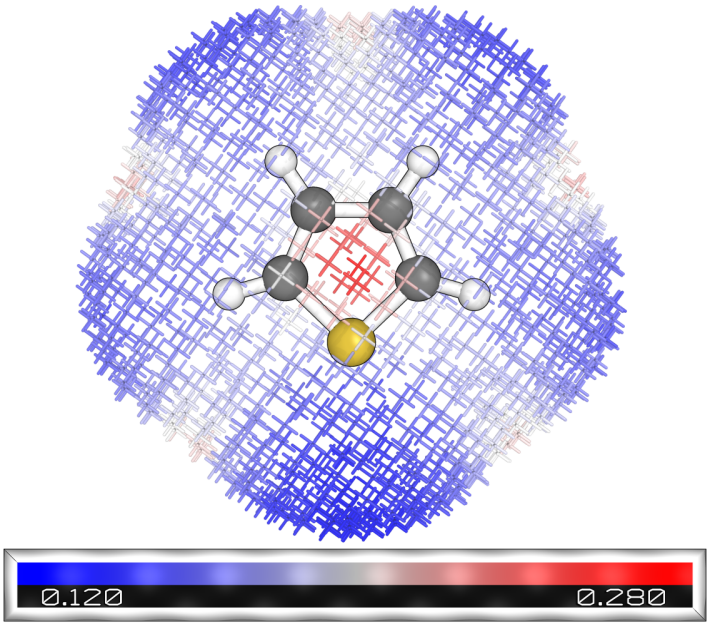



Figure S59: Benchmark dispersion map from dDsC with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

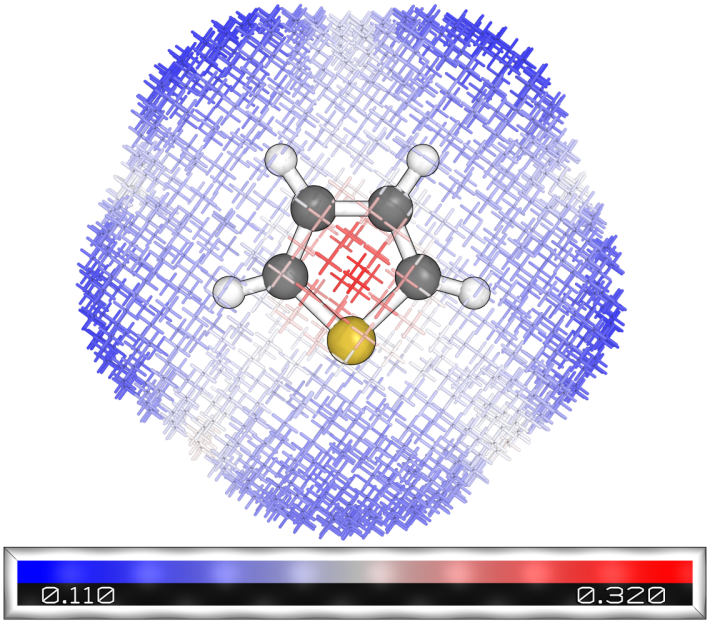



Figure S60: Benchmark dispersion map from VV10 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

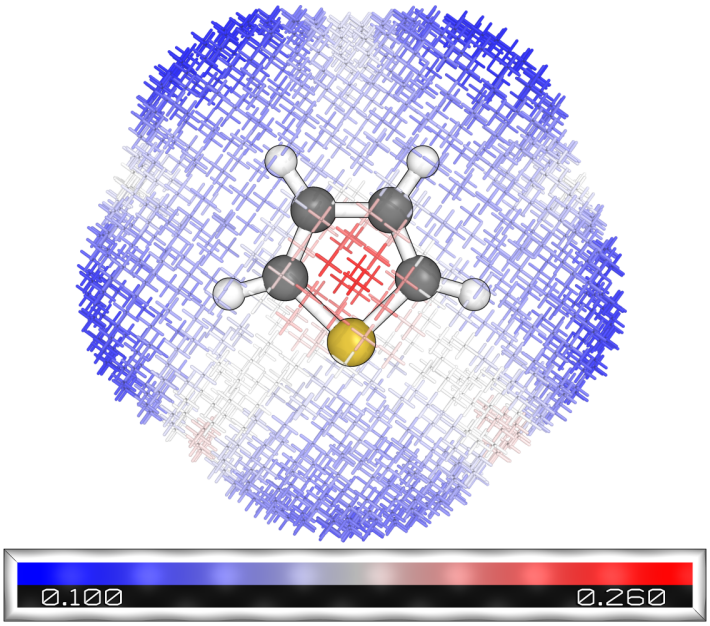



Figure S61: Benchmark dispersion map from XDM with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

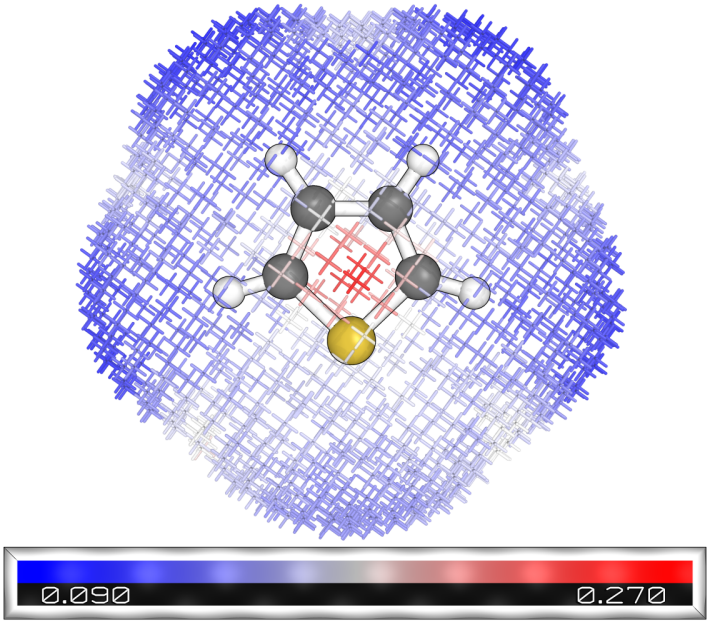



Figure S62: Benchmark dispersion map from LED with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

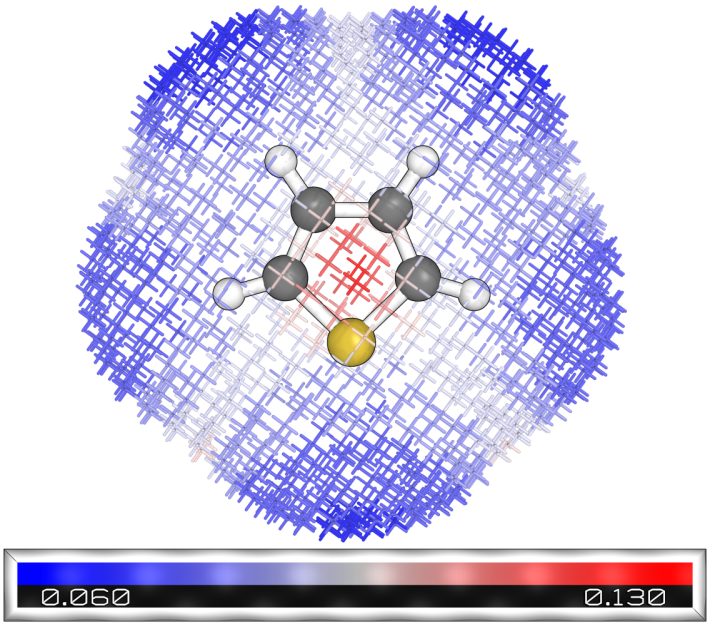



Figure S63: Benchmark dispersion map from sSAPT0 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

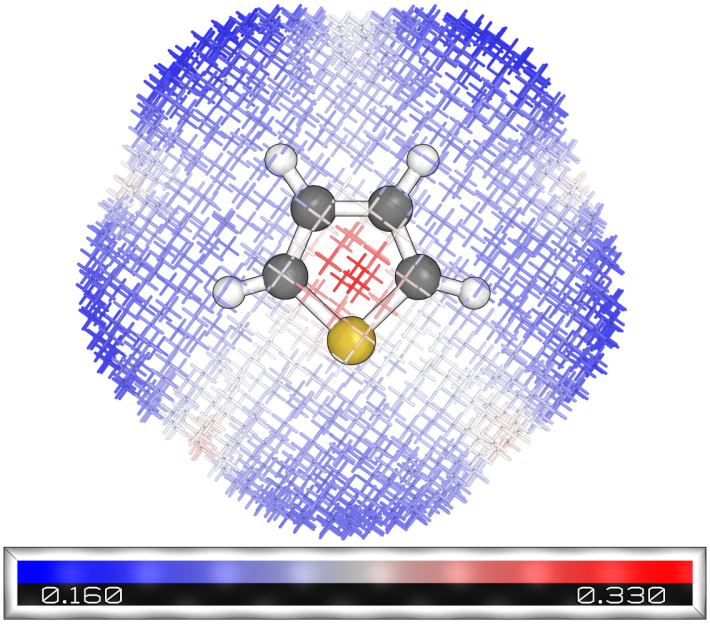



Figure S64: Benchmark dispersion map from SAPT2+ with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

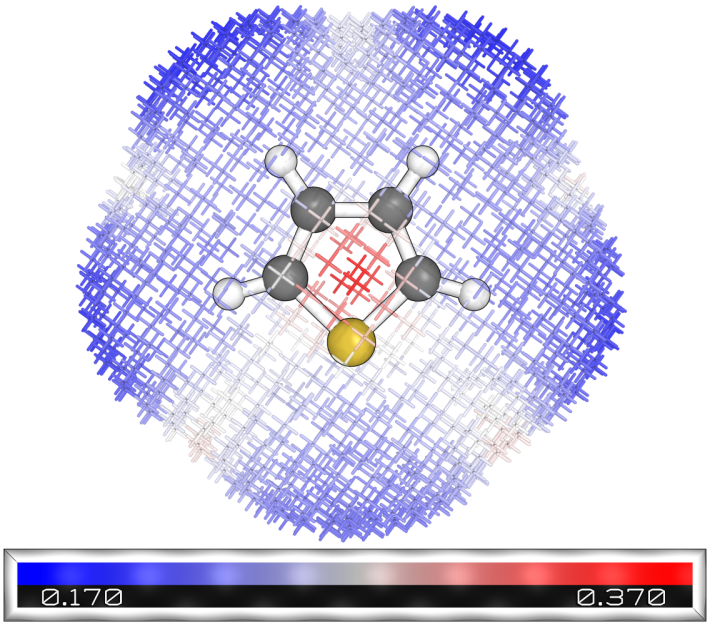



Figure S65: Benchmark dispersion map from SAPT2+(3) with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

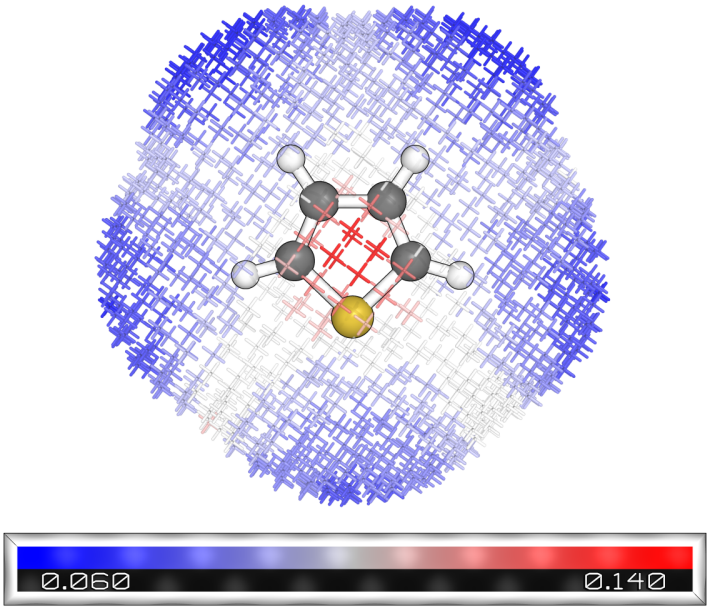



Figure S66: Benchmark dispersion map from sSAPT0 with Ne (at $1 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

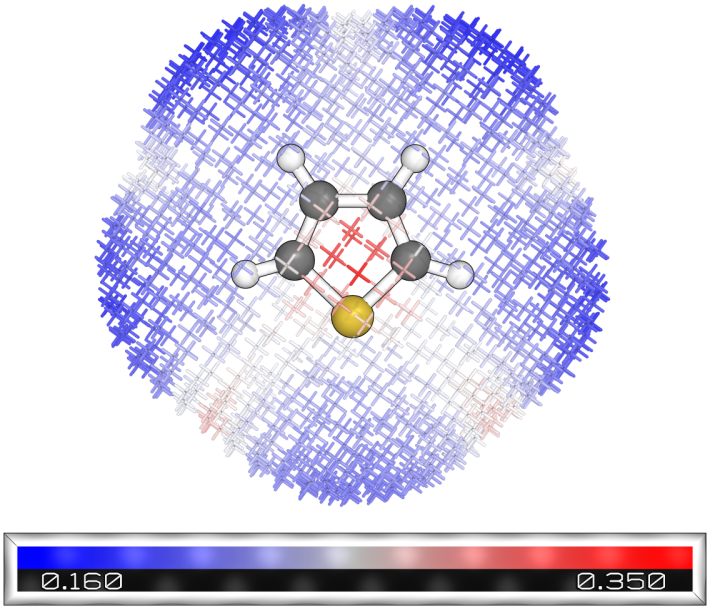



Figure S67: Benchmark dispersion map from SAPT2+ with Ne (at $1 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

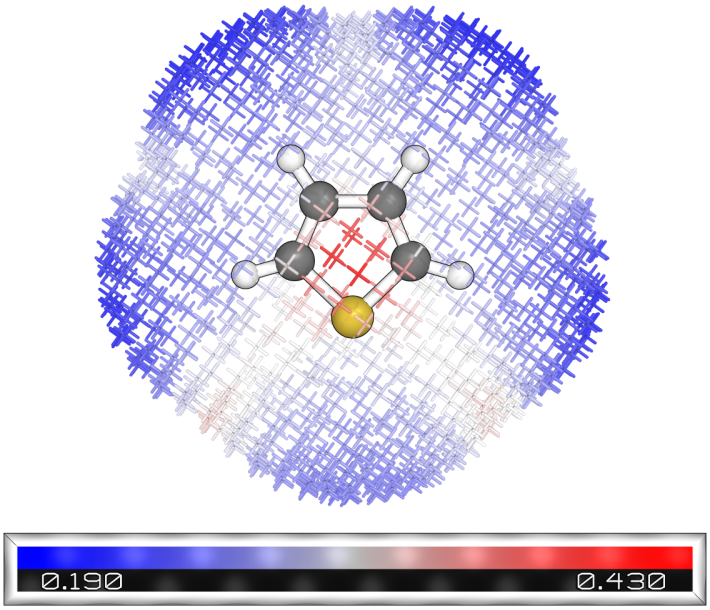



Figure S68: Benchmark dispersion map from SAPT2+(3) with Ne (at $1 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

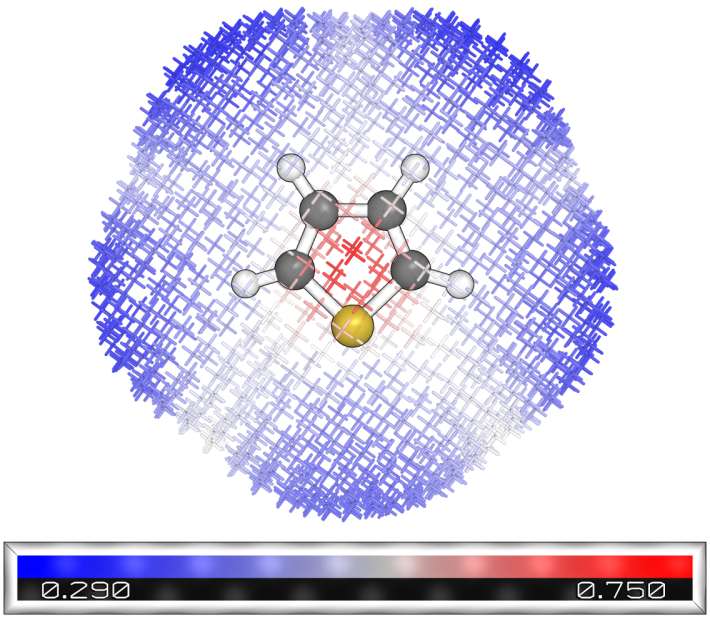



Figure S69: Benchmark dispersion map from sSAPT0 with Ar (at $5 \cdot 10^{-7}\,\mathrm{e\,Bohr^{-3}}$).

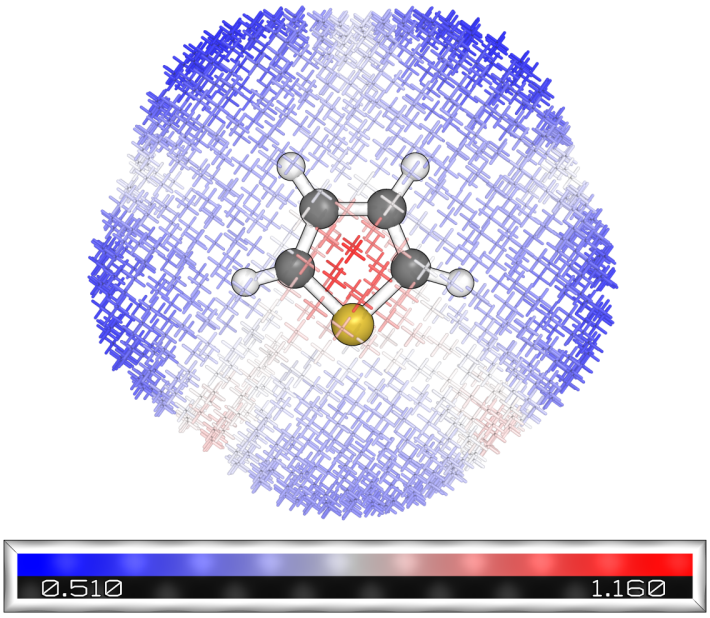



Figure S70: Benchmark dispersion map from SAPT2+ with Ar (at $5 \cdot 10^{-7}\,\mathrm{e\,Bohr^{-3}}$).

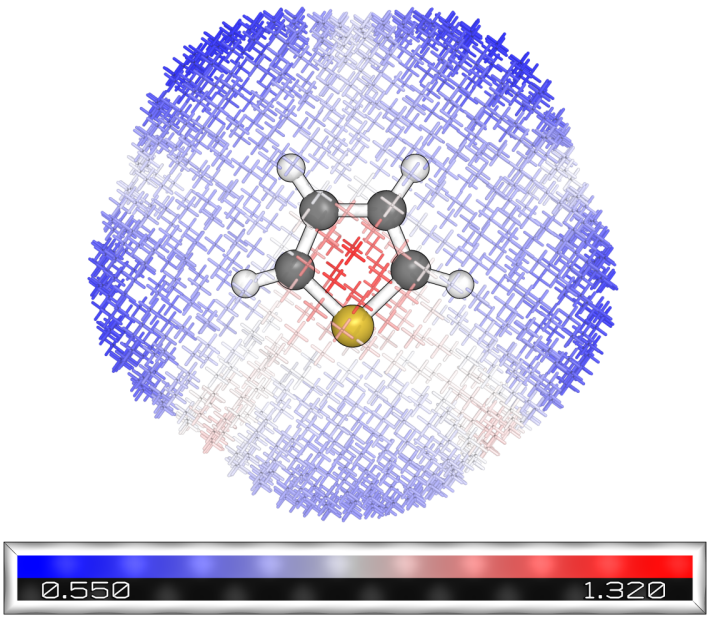



Figure S71: Benchmark dispersion map from SAPT2+(3) with Ar (at $5 \cdot 10^{-7}\,\mathrm{e\,Bohr^{-3}}$).

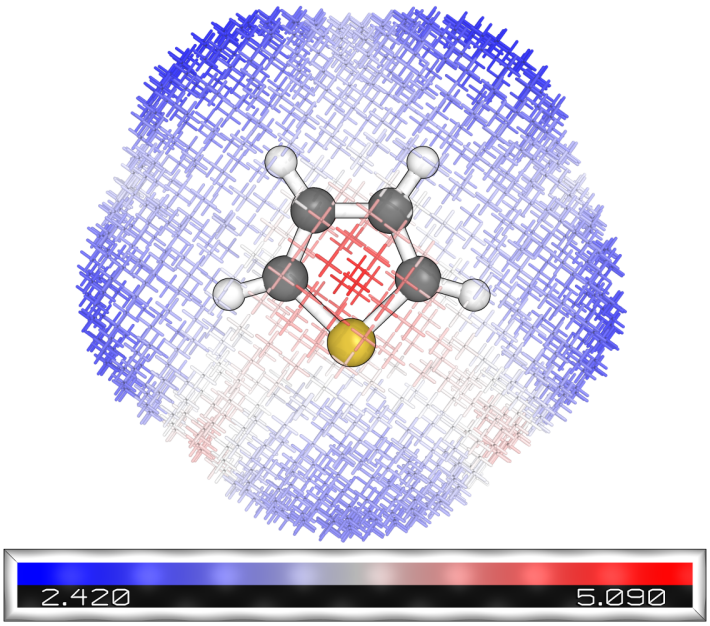



Figure S72: Sparse LDP map with D3 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

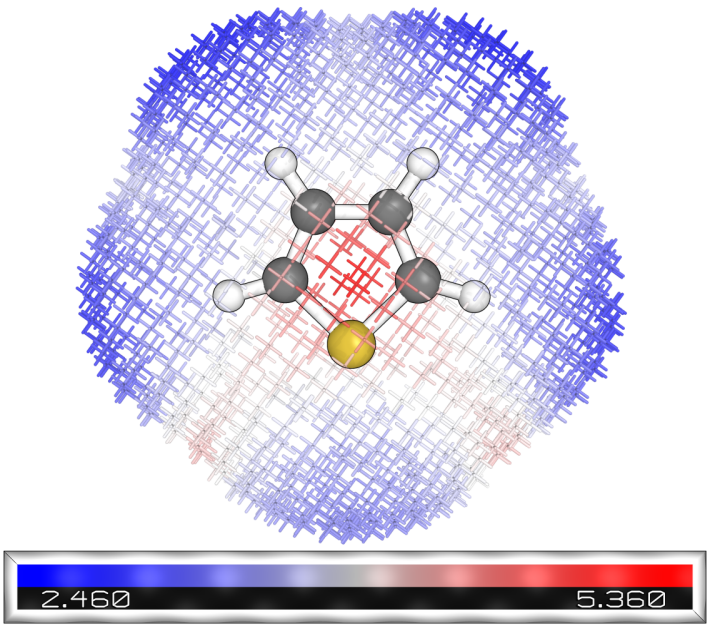



Figure S73: Sparse LDP map with D4 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

**Selenophene**

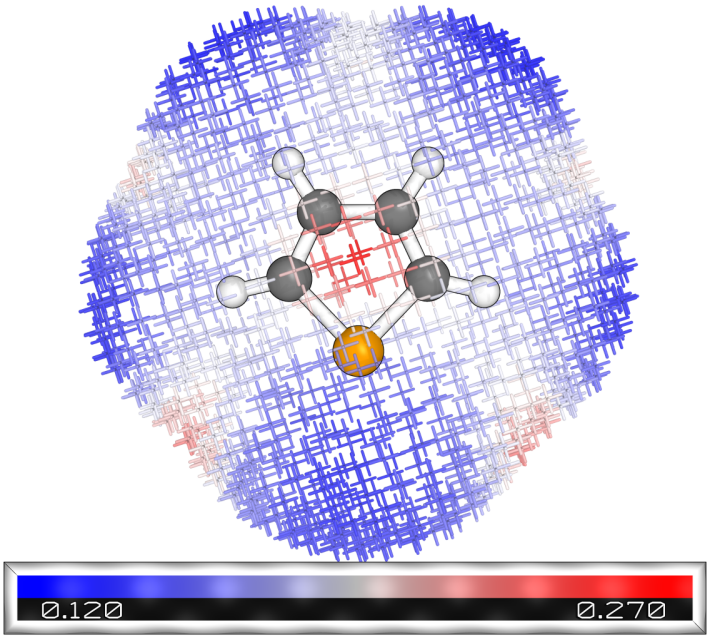



Figure S74: Benchmark dispersion map from D3 with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

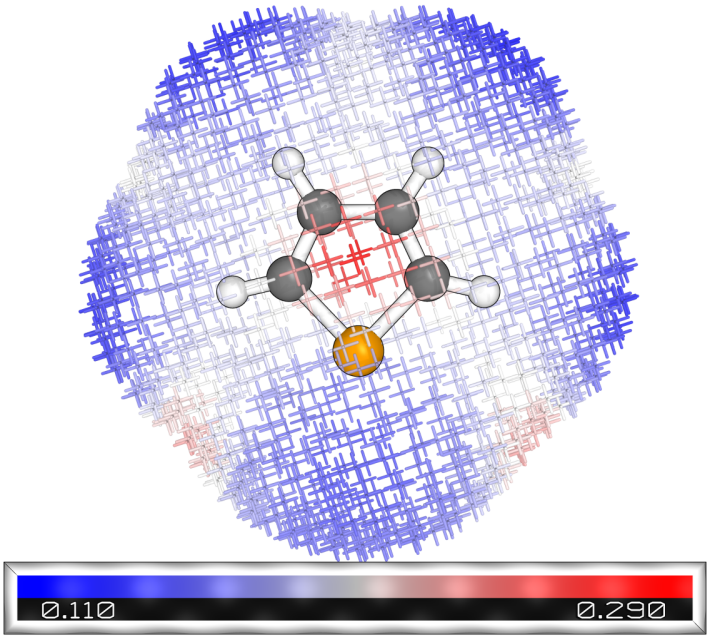



Figure S75: Benchmark dispersion map from D4 with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

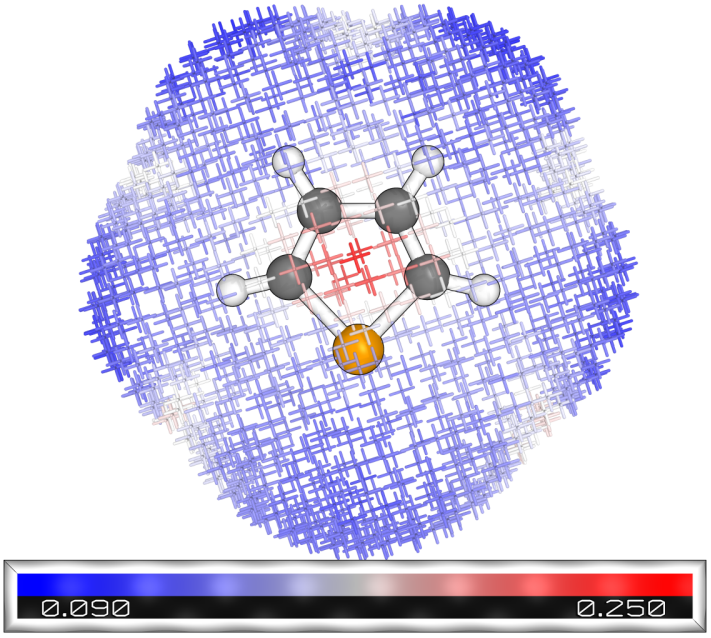



Figure S76: Benchmark dispersion map from LED with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

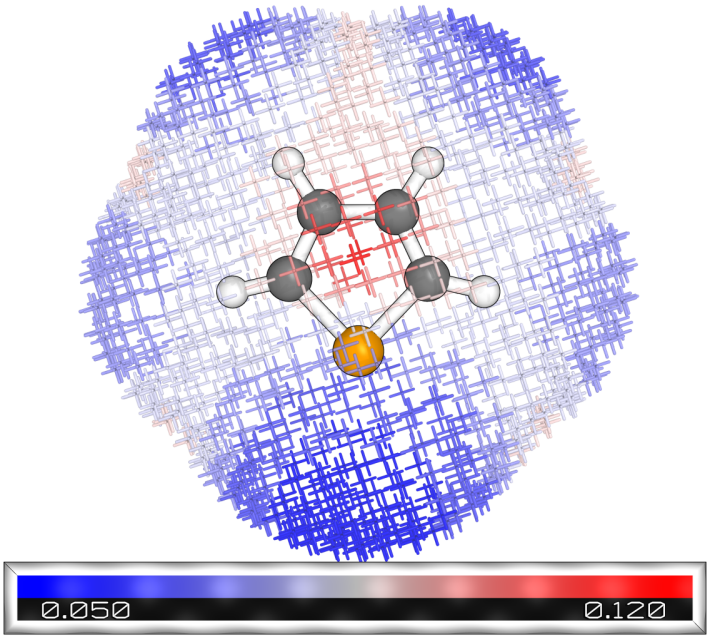



Figure S77: Benchmark dispersion map from sSAPT0 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

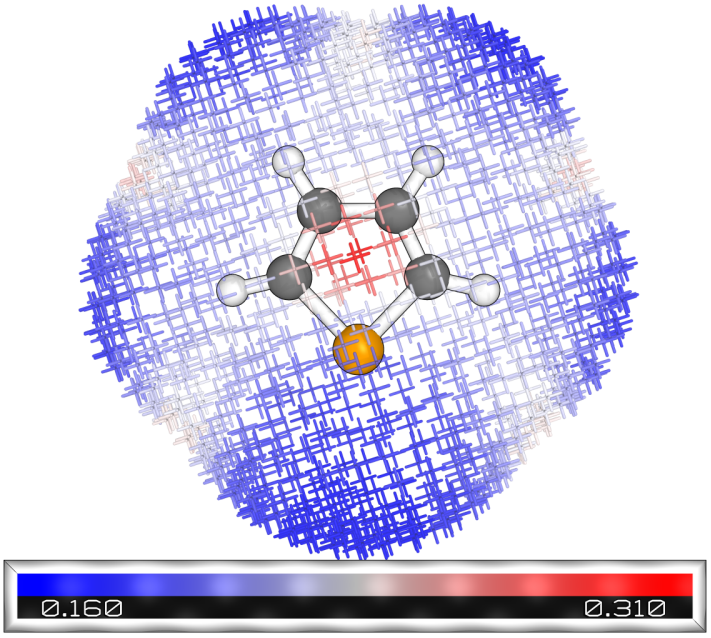



Figure S78: Benchmark dispersion map from SAPT2+ with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

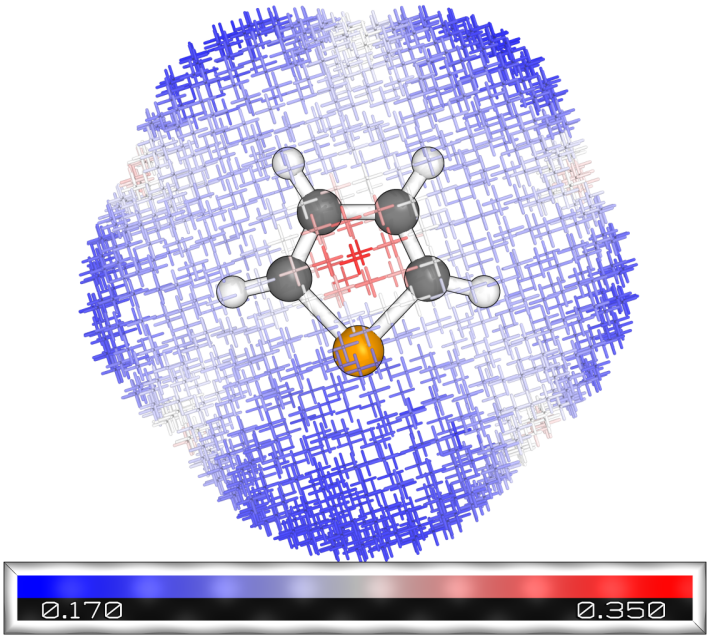



Figure S79: Benchmark dispersion map from SAPT2+(3) with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

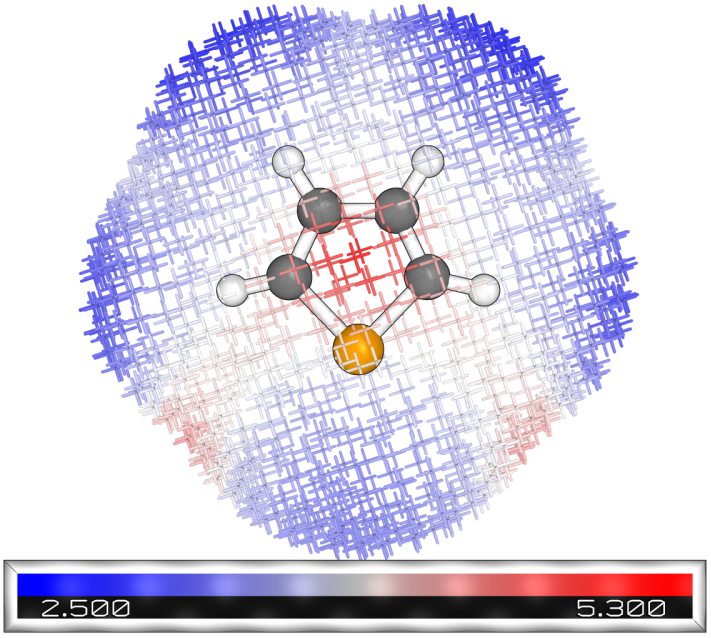



Figure S80: Sparse LDP map with D3 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

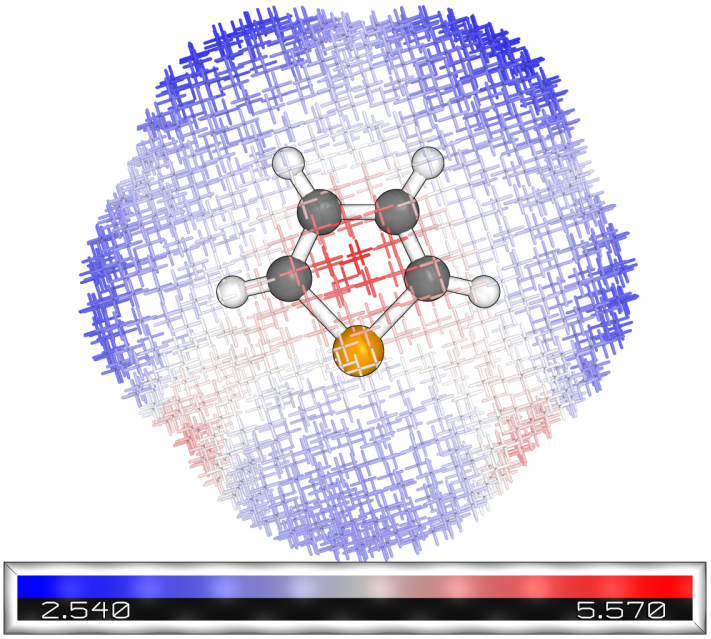



Figure S81: Sparse LDP map with D4 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

**Tellurophene**

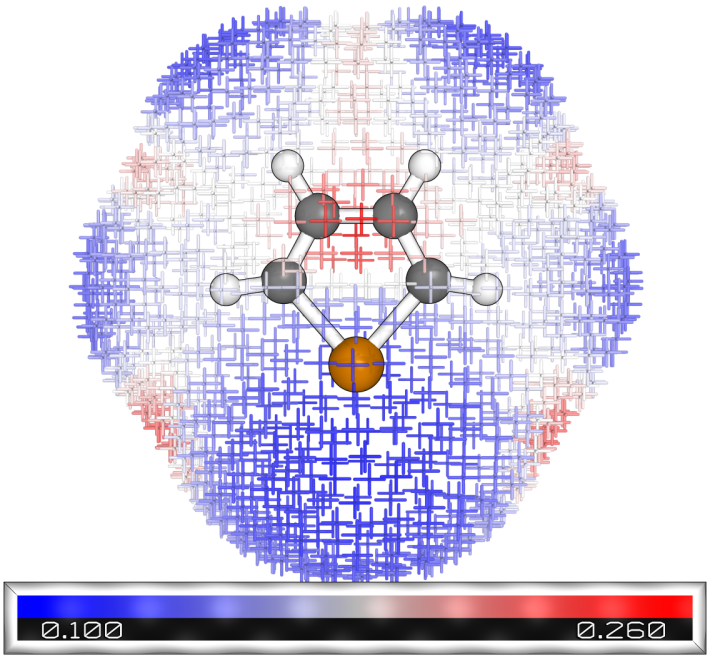



Figure S82: Benchmark dispersion map from D3 with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

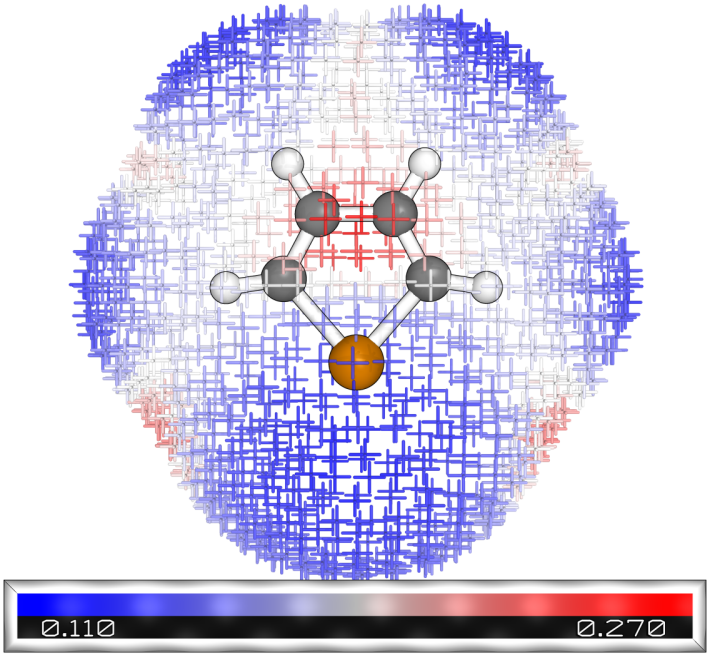



Figure S83: Benchmark dispersion map from D4 with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

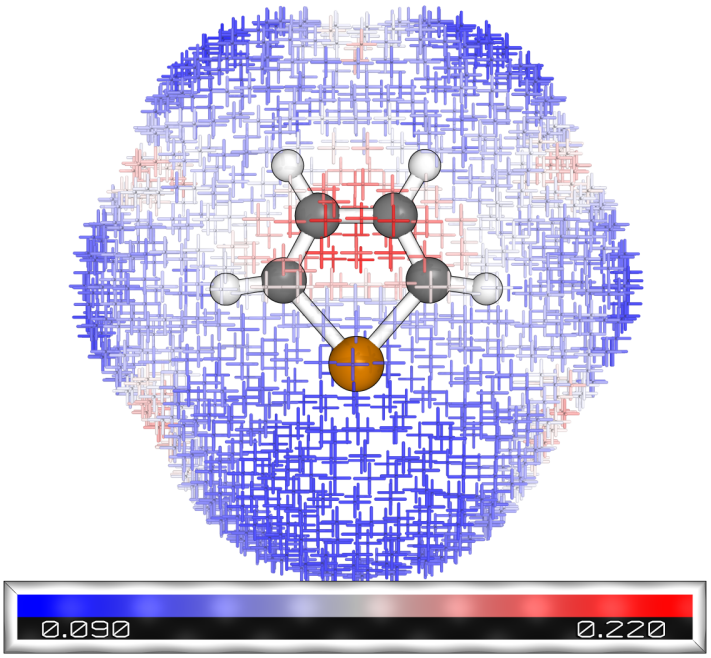



Figure S84: Benchmark dispersion map from LED with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

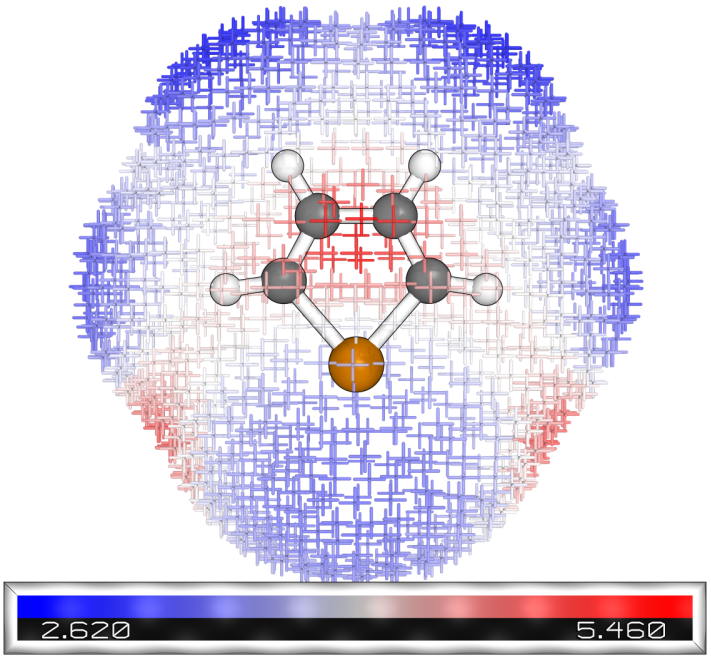



Figure S85: Sparse LDP map with D3 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

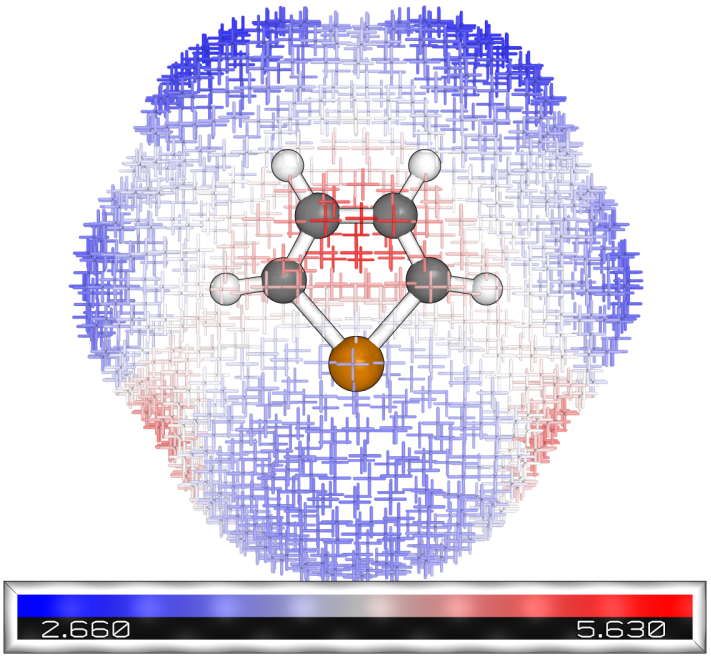



Figure S86: Sparse LDP map with D4 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

**Cu(I) N-heterocyclic carbene**

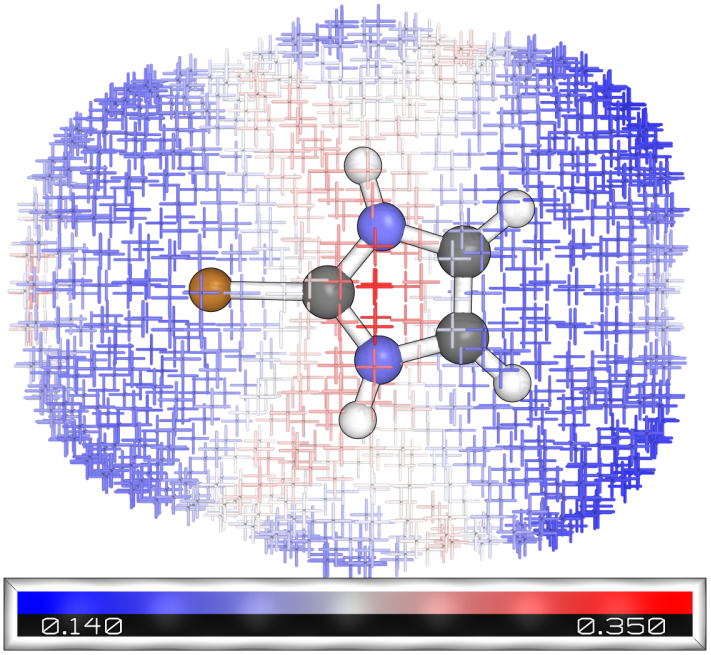



Figure S87: Benchmark dispersion map from D3 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

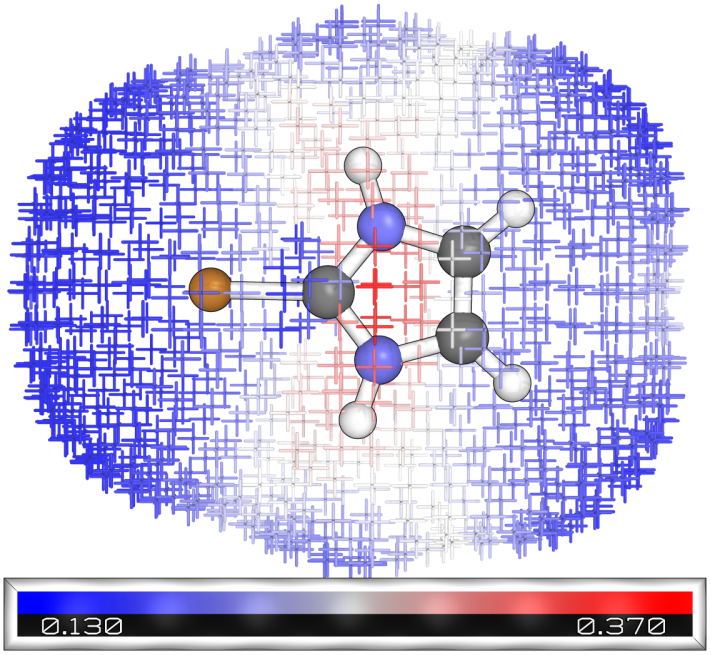



Figure S88: Benchmark dispersion map from D4 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

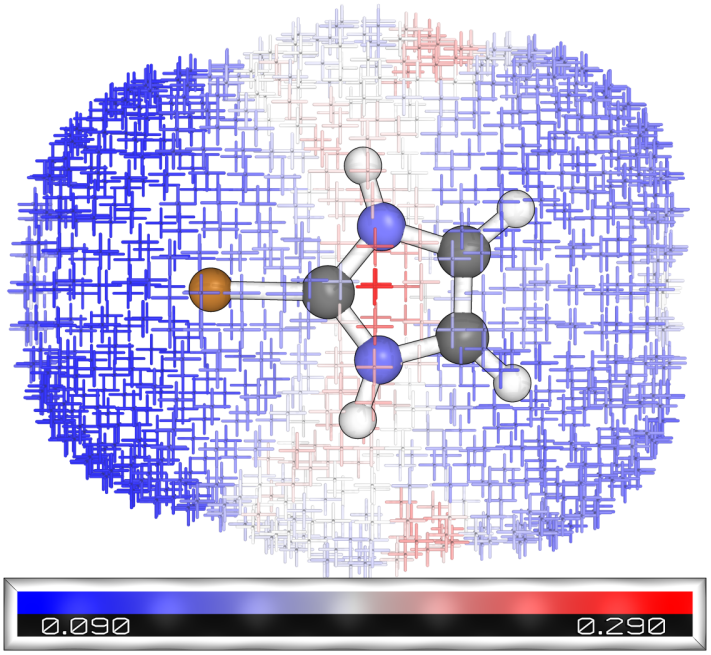



Figure S89: Benchmark dispersion map from LED with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

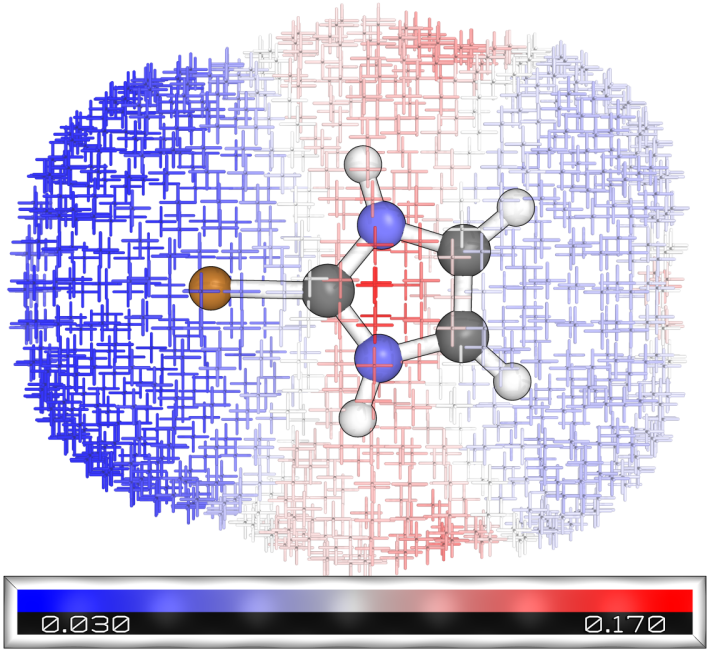



Figure S90: Benchmark dispersion map from sSAPT0 with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

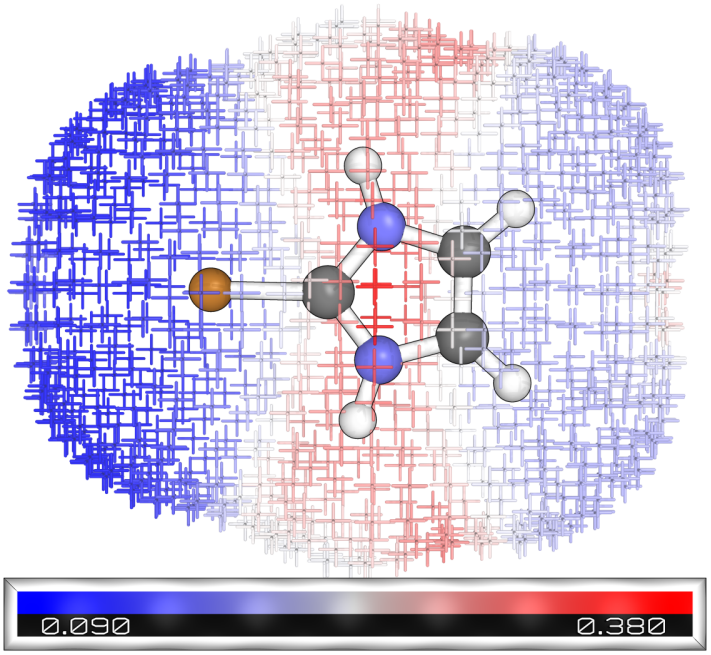



Figure S91: Benchmark dispersion map from SAPT2+ with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

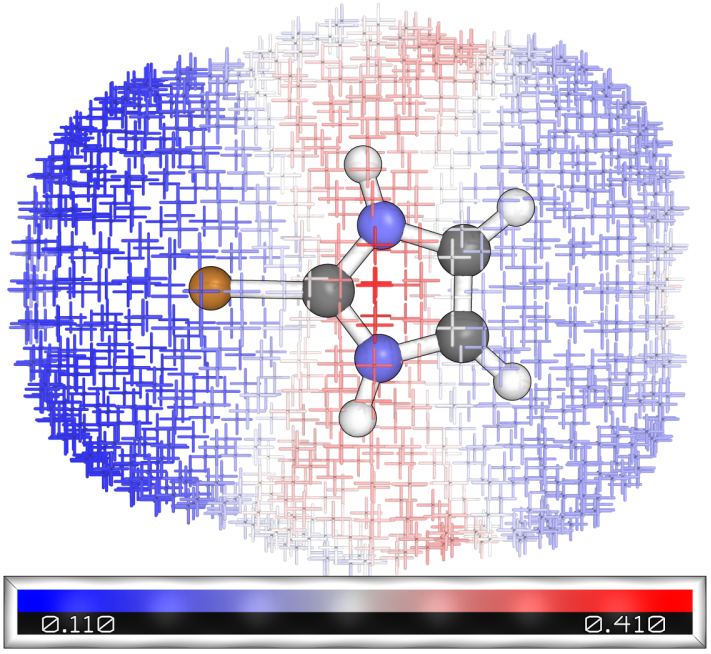



Figure S92: Benchmark dispersion map from SAPT2+(3) with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

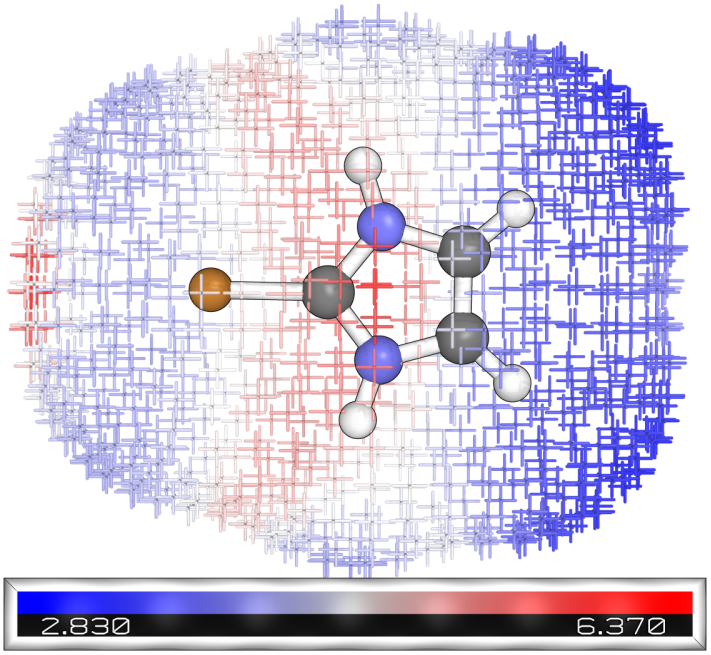



Figure S93: Sparse LDP map with D3 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

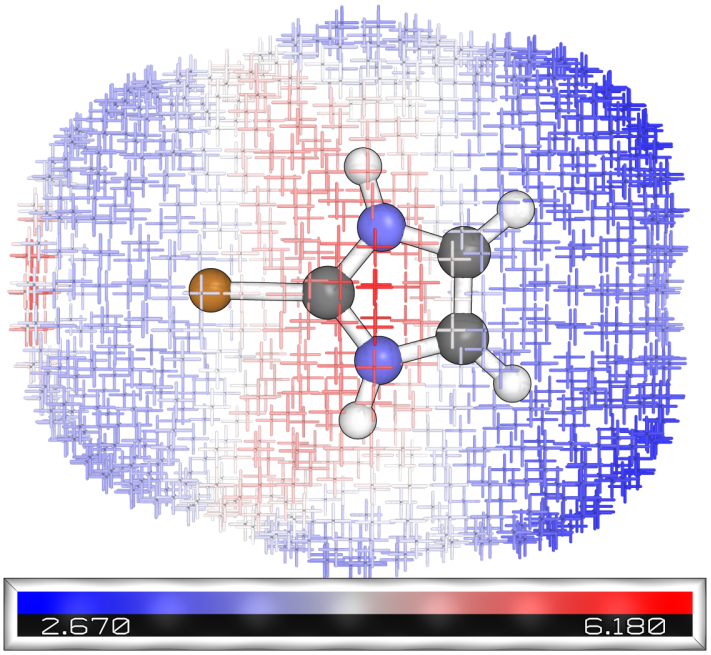



Figure S94: Sparse LDP map with D4 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

**Pd(II) diimine**

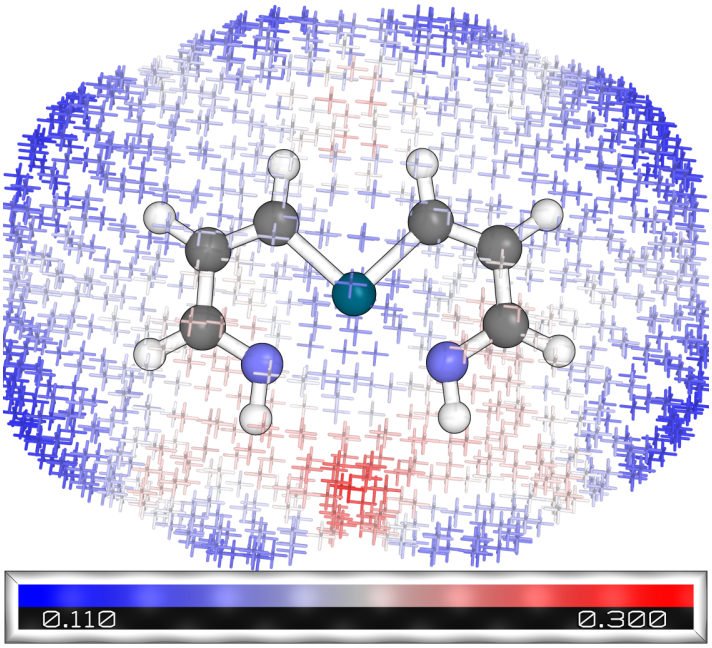



Figure S95: Benchmark dispersion map from D3 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

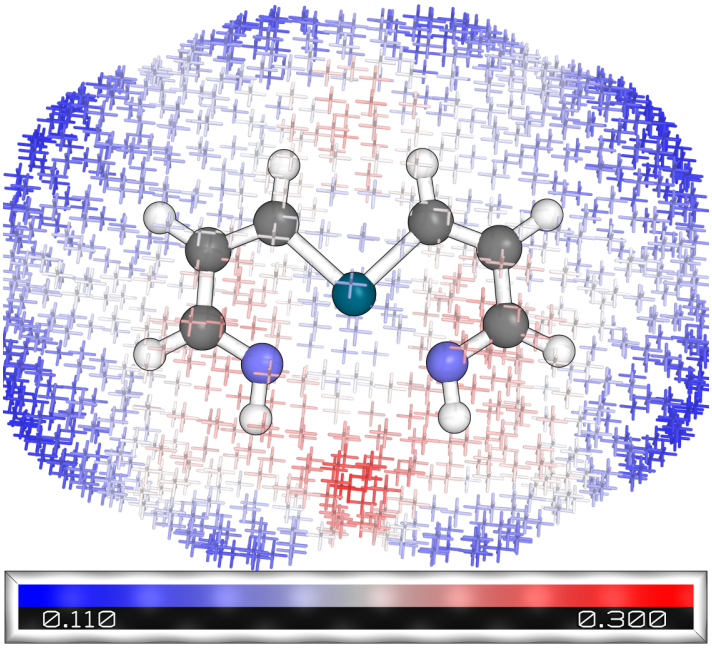



Figure S96: Benchmark dispersion map from D4 with He (at $5 \cdot 10^{-6}$ e Bohr$^{-3}$).

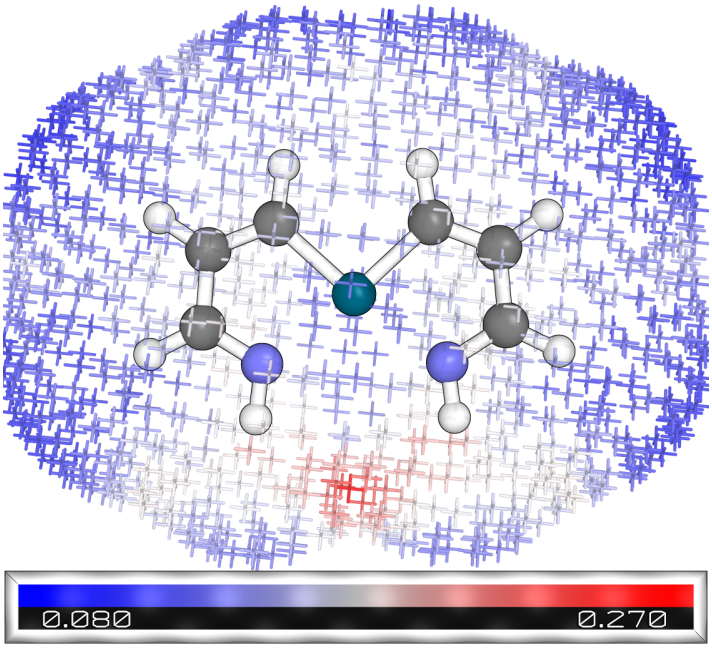



Figure S97: Benchmark dispersion map from LED with He (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

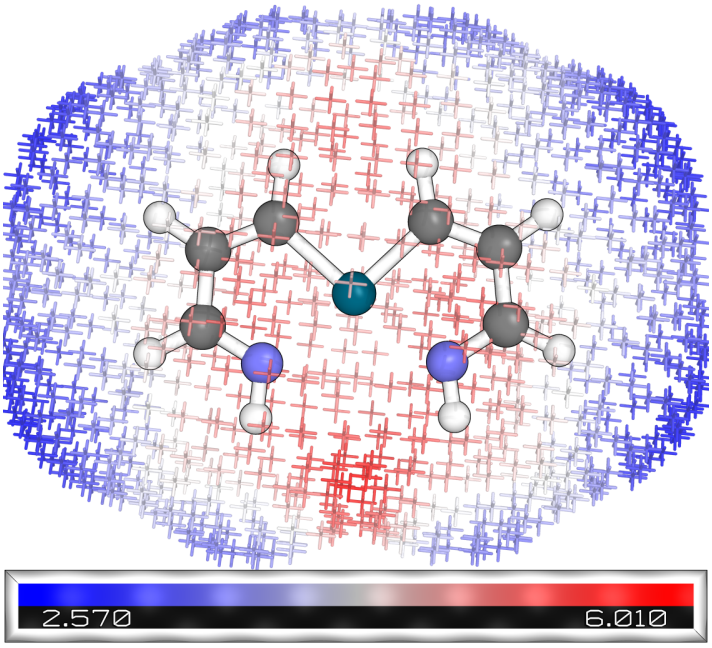



Figure S98: Sparse LDP map with D3 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

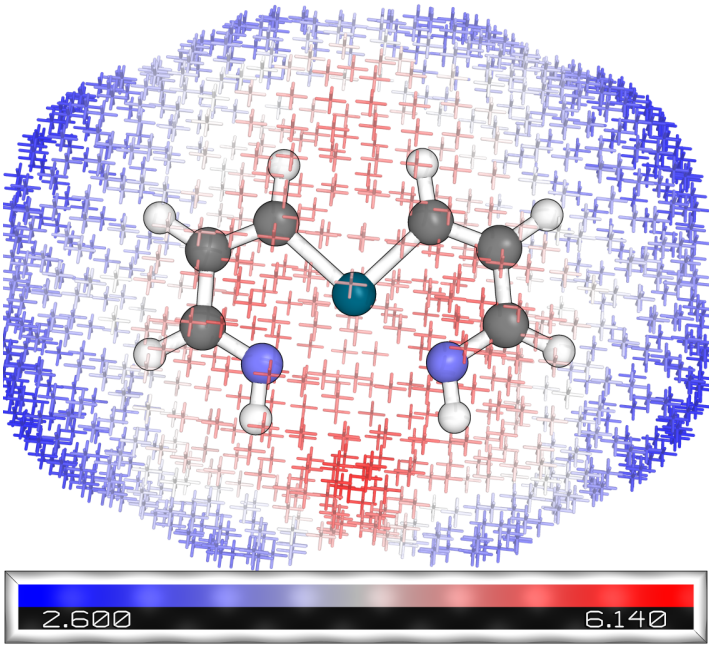



Figure S99: Sparse LDP map with D4 (at $5 \cdot 10^{-6}\,\mathrm{e\,Bohr^{-3}}$).

### 2.1.3 Case Studies

**NCIs in Small Molecules** Next, we looked into comparing the LDP maps of propane and perfluoropropane (cf. Figure S100). A recent study showed that the differences in the properties of alkanes and perfluoroalkanes can be explained by their dispersive abilities and their interaction geometries.[70] Their LDP maps reveal that the corresponding maxima are at distinct positions. While the maximum, for propane, is orthogonal to the plane of the carbon atoms, for perfluoropropane, it is in the plane going through the carbon atoms. Notably, the newly defined $P_{int}$ using D4 correctly reproduces that perfluoropropane ($P_{int} = 13.8\,\mathrm{kcal^0\,5\ mol^{-}0\,5}$) has a higher intrinsic dispersive ability than propane ($P_{int} = 13.1\,\mathrm{kcal^0\,5\ mol^{-}0\,5}$).[70] Based on the LDP maps one would expect the most stable conformers of the respective dimers to be different and high level computations indeed confirm that.[70] Propane dimer prefers the conformer resulting from inversion and consecutive translation orthogonal to the carbon atoms plane, perfluoropropane dimer prefers the conformer resulting from inversion and consecutive translation in the carbon atoms plane.[70] The corresponding structures are depicted

in Figure S100 with intermolecular LDP maps to compare the dispersive contacts. While the LDP maximum of the isolated molecules has a higher value in perfluoropropane, the LDP maximum on the intermolecular Becke surface has a higher value in propane. This goes in line with the poor interaction geometries of linear perfluoroalkanes compared to their alkane analogues.[70] Hence, the LDP maps correctly characterize the differing spatial preferences of alkanes and perfluoroalkanes to interact by dispersion.

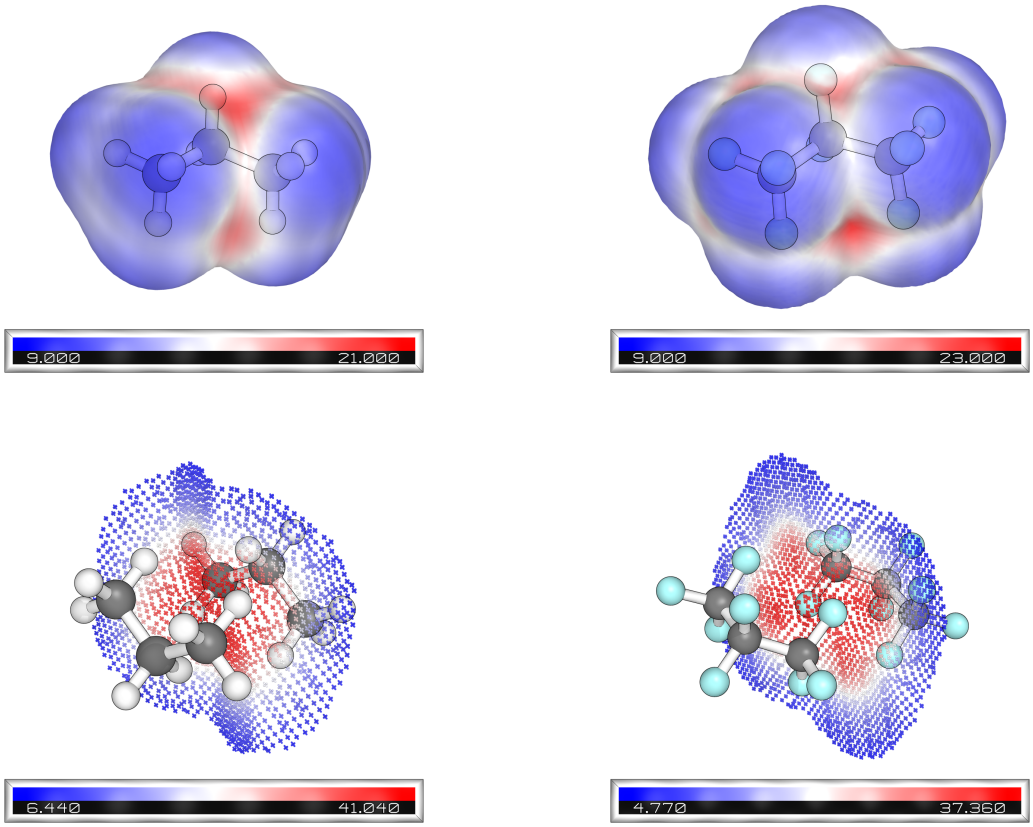



Figure S100: Investigation of the vdW dimers of propane and perfluoropropane. Full LDP map of propane (top left) and perfluoropropane (top right) from D4 (at $1 \cdot 10^{-3}$ e Bohr$^{-3}$). LDP mapped onto the intermolecular Becke surface of the most stable dimers of propane (bottom left) and perfluoropropane (bottom right).

Additionally, the LDP of bromine was computed to benchmark it against interaction maps from higher level of theory provided in the literature.[71] The corresponding result is

depicted in Figure S101. The positions of the local extrema are the same as in the benchmark methods. Notably, the maxima collinear with the covalent bond have approximately the same P value as the maxima around the center of the molecule indicating a slight underestimation of the former compared to benchmark results, which can be rationalized by the neglect of three-body dispersion in our P parameter.

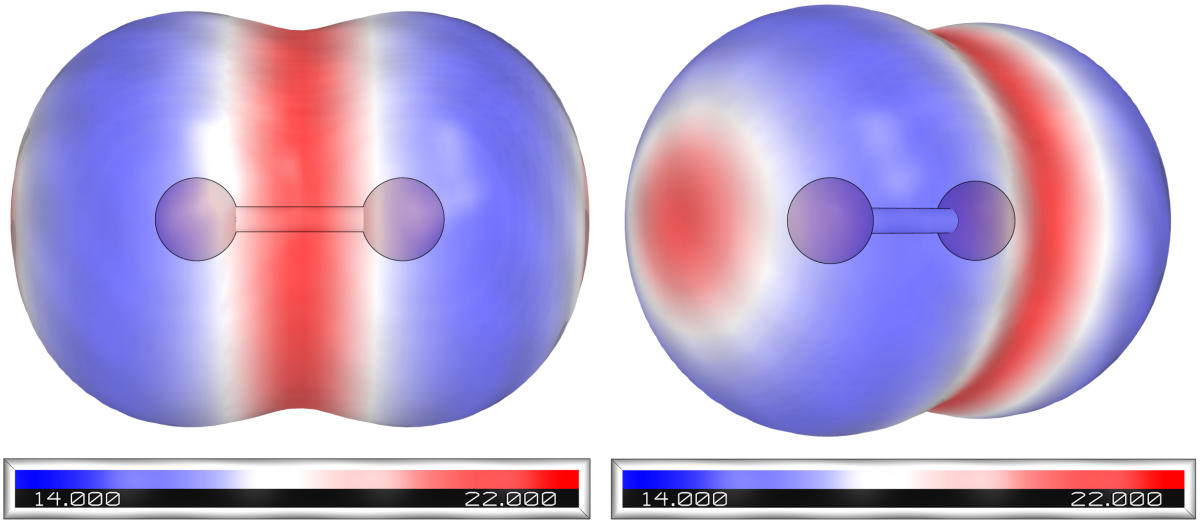
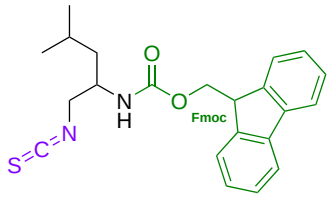



Figure S101: Two perspectives of the full LDP map of bromine from D4 (at $1 \cdot 10^{-3}$ e Bohr$^{-3}$).

**Chalcogen Bonding** In addition to the 2Z-2N squares discussed in the main text, we also investigated chalcogen bonding in an isothiocyanate[72] derivative of fluorenylmethyloxycarbonyl-protected leucin (Fmoc-Leu-NCS, Scheme 1).




Scheme 1: Fmoc-Leu-NCS.

To look into the importance of dispersion in the close S-N contact compared to close CH-π contacts observed in the crystal structure of Fmoc-Leu-NCS, we computed a dispersion potential (DP) Becke maps between two molecules in the crystal structure (S103). The corresponding results were compared to Becke maps of the normalized contact distances (S102), to intermolecular NCI plots (S104) and to DID plots (S105). First, it can be seen again that the LDP Becke map is much more specific in highlighting interactions compared to the $d_{norm}$ Becke map. While the $d_{norm}$ Becke map reveals a broad range of close contacts, only two regions are highlighted in the LDP Becke maps. The region of strongest intermolecular dispersion corresponds to the contact between the iso-butyl group and the fluorenyl group. Additionally, the close S-N contact also shows a significant amount of dispersion indicating again that chalcogen bonding can be reinforced by a significant amount of dispersion. Furthermore, the relative (dispersive) strength of the contacts can be estimated easier by the LDP maps compared to both the NCI plots and the DID plots. The NCI plots show an overall attractive interaction for the close S-N contact. However, the close CH-π contact between the iso-butyl group and the fluorenyl group shows both attractive and repulsive regions making it not straightforward to assess whether this contact is overall attractive, and if so, how strong. Moreover, the DID plots reveal the same interactions as contributing most to the intermolecular dispersion showing that the LDP Becke map is a simple and robust

way to assess dispersive interactions.

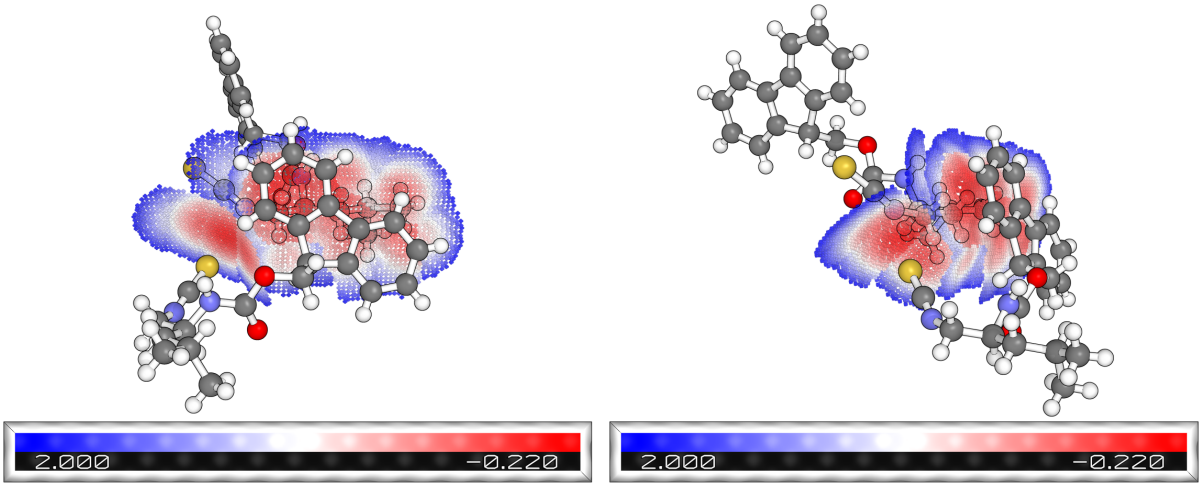



Figure S102: Normalized contact distance ($d_{norm}$) projected onto the Becke surface of two molecules of Fmoc-Leu-NCS depicted from two perspectives.

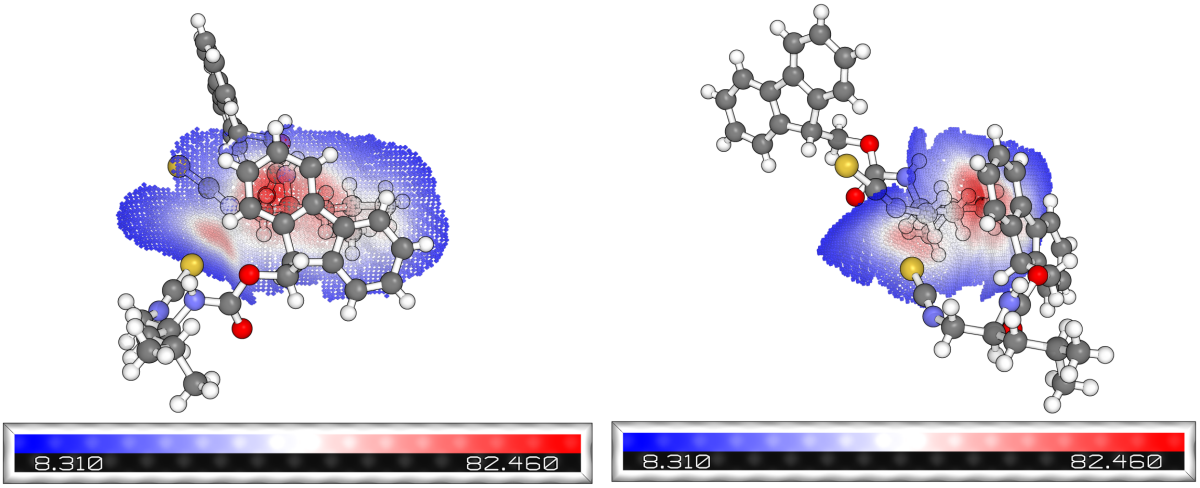



Figure S103: LDP projected onto the Becke surface of two molecules of Fmoc-Leu-NCS depicted from two perspectives.

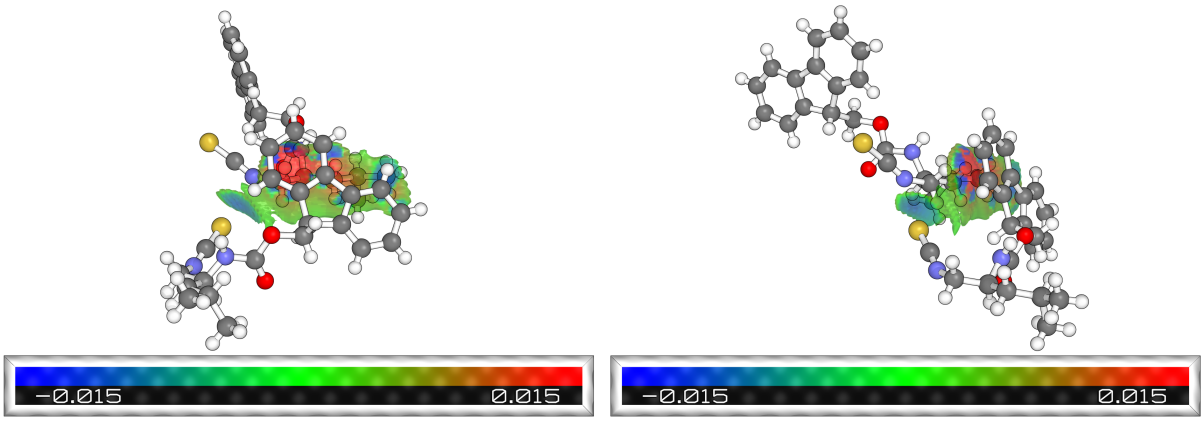



Figure S104: Intermolecular NCI plot of two molecules of Fmoc-Leu-NCS depicted from two perspectives.

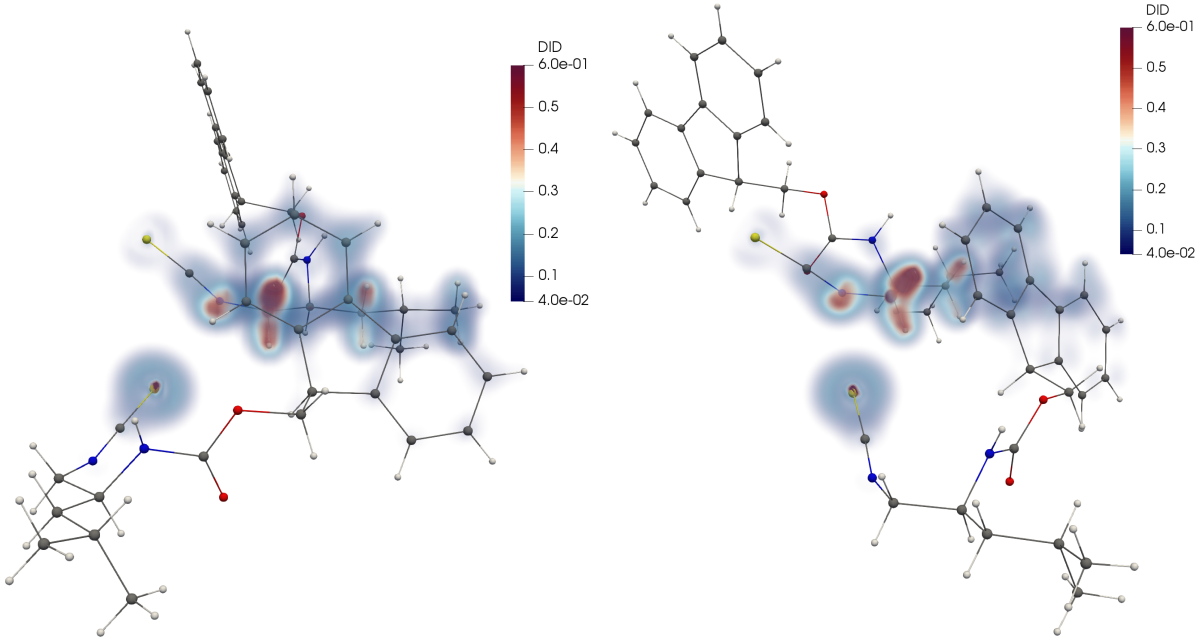



Figure S105: DID plot of two molecules of Fmoc-Leu-NCS depicted from two perspectives.

**Organometallic Chemistry** Additionally, the $P_{int}$ of the elements can be used to estimate the dispersive strength of Au-Au contacts compared to Cu-Cu and Ag-Ag contacts. The estimated relative strengths is Cu-Cu $\approx$ Ag-Ag ¿ Au-Au, which is qualitatively in line with high level computations despite unaccounted non-dispersive contributions.[73,74] Hence, our new simple tools can be used to understand magnitudes and trends of the dispersive component of metallophilic interactions.

**Catalysis** We also present additional results for the multiple linear free energy relationship (MLFER) example presented in the main text (Figure 13). Figure S106 shows the fitting results without including the outlier from the literature. While the fitting remains approximately equally good, the robustness as indicated by the leave-one-out (L1O) measure increases. Figure S107 shows the most significant single parameter fits of the corresponding models with including the outlier from the literature. The most significant single parameter in each of the two approaches is the product of the $NBO_{C1}$ charge and the respective dispersion parameter used ($P_{int}$ or the product of $P_{int}$ and $A_{rel}$, respectively). The product of $P_{int}$ and $A_{rel}$ shows a somewhat more robust single parameter correlation as shown by the significantly better L1O measure.

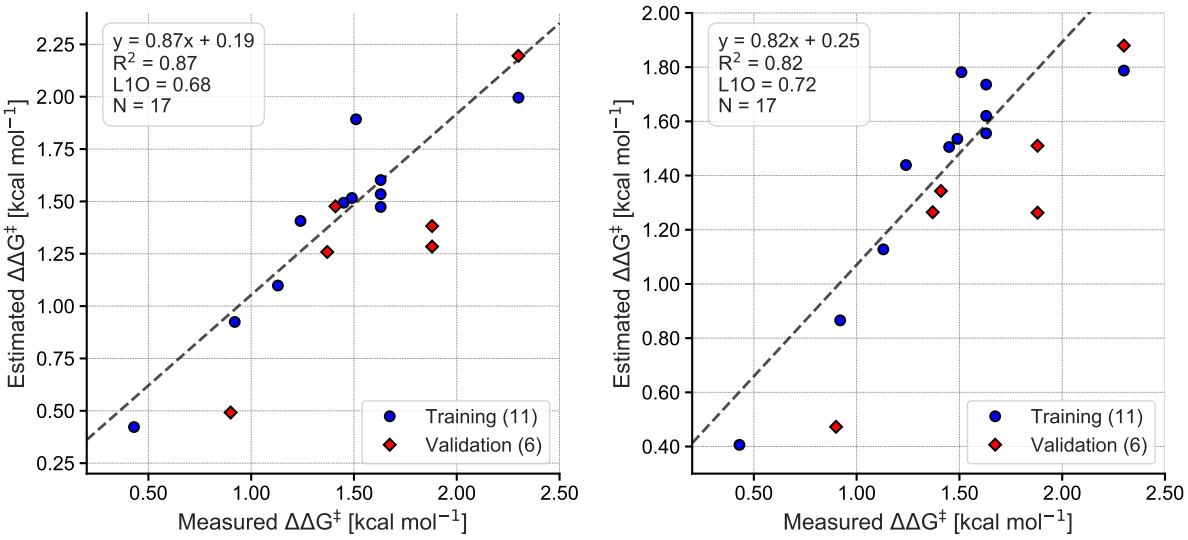



Figure S106: MLFER analysis of Pd-catalyzed enantioselective 1,1-diarylation of benzyl acrylates using $P_{int}$ (a) and the product of $P_{int}$ and $A_{rel}$ (b) to replace ${}^{S}E_{\pi}$ from the original model with potential outlier removed from the model.

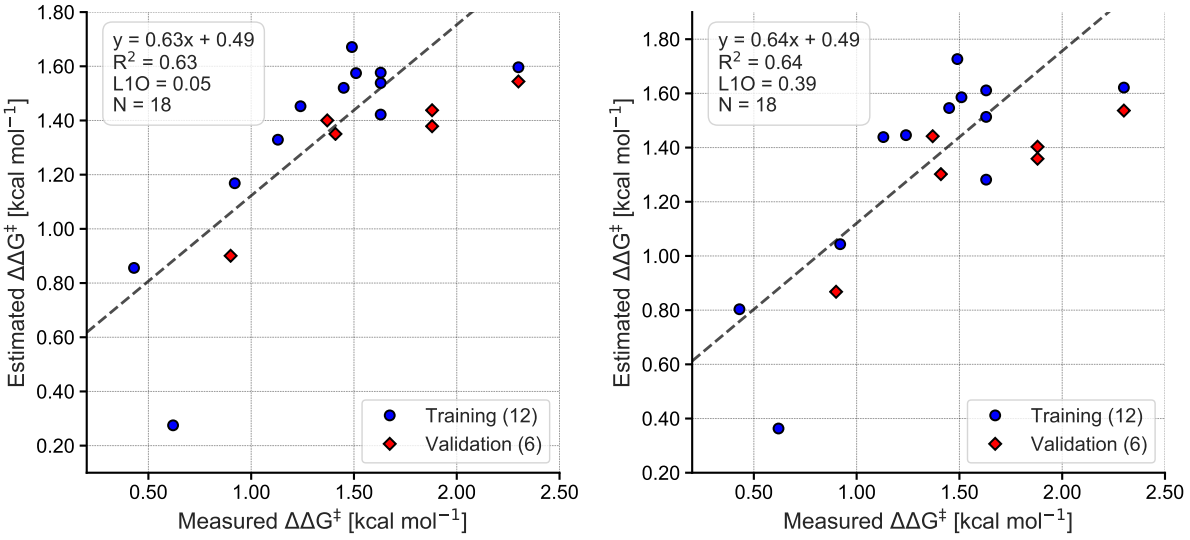



Figure S107: Single parameter correlation analysis of Pd-catalyzed enantioselective 1,1-diarylation of benzyl acrylates using the product of $NBO_{C1}$ and $P_{int}$ (a) and the product of $P_{int}$ and $A_{rel}$ (b) as most significant parameters.

## 2.2 Discussion

In this section additional discussion, that did not fit into the main manuscript, is provided. By using the sum of $C_6$ and $C_8$ coefficients (Equation 3), the product of two P values does not only lead to $C_6$ and $C_8$ energy terms, but also to an effective $C_7$ cross term with a distance dependence of $R^{-7}$. This leads to an artificial overestimation of the resulting interaction energy. However, as we neglect higher order dispersion coefficients and do not implicitly account for them by introducing empirical scaling factors, which are typically employed in dispersion corrections,[75] this effectively recovers part of the neglected higher order energy terms.[75] Notably, in molecules, due to anisotropy, $C_7$ dispersion coefficients are non-zero and can account for several percent of the total dispersion providing some physical justification for this term.[76] Furthermore, the additional energy contribution is only relevant at short distances because of its higher-order distance dependence. Hence, there is some physical justification for the presence of this cross term.

In addition, at short distances, i.e. typically significantly shorter than the sum of the

vdW radii, the long range asymptotic dispersion energy formula (Equation 3) is not a good approximation anymore and results in significant overestimation of dispersion. By neglecting higher-order dispersion coefficients, this overestimation is somewhat alleviated and the P value remains at least a semi-quantitative measure of dispersive interaction potential in that distance regime. In dispersion correction schemes, this is usually accounted for by using damping functions like Becke-Johnson damping.[59] However, as the P measure is designed to describe mid- to long-range dispersion adequately, the use of damping functions is not necessary and, for the sake of simplicity, we decided not to use them.

We also compared the projection of the normalized contact distance[77] to the projection of LDP on Becke surfaces (Figure 7). These case studies demonstrate that the LDP projection is more specific than just indicating atoms at close distances and provides a good measure of relative strength of dispersive interactions as the results agree qualitatively well with DID plots. Notably, LDP Becke maps do not use the actual interaction distances but rather the respective distances to the Becke surface. This results in overestimated P values and an increased relative weight of the $C_8$ term relative to the $C_6$ term. Therefore, P values on Becke surfaces are merely semi-quantitative measures of dispersion with the advantage that it leads to a better distinction of the respective contact strength.

In the table of common organic substituents (Table 1) and in the MLFER models (Figure 13), we used both $P_{int}$ alone and the product of $P_{int}$ and the surface area ($A_{rel}$) for the description of the LDP of a group or molecule. These two parameters describe different dispersive properties. $P_{int}$ is a measure of the average strength of one dispersive contact. When multiplied with the surface area, it becomes a measure of how much dispersion the group or molecule can provide in total. Hence, it is also a measure of how many dispersive contacts it can have. Table 1 shows that there is some correlation between the two parameters. However, they are not equivalent suggesting that, depending on the application at hand, one or the other is more appropriate.

# 3 Computational Raw Data

In this section, computational results are provided in tables and the corresponding contents are explained briefly.

## 3.1 Dispersion Scale

Tables S4 and S5 contain the atomic radii,[78] homoatomic $C_6$ and homoatomic $C_8$ dispersion coefficients from D4 of all the elements that were used to construct the periodic table of the elements with $P_{int}$. The homoatomic $C_6$ and $C_8$ dispersion coefficients of cerium (Ce) are outliers and were not used. This is apparent when looking at the reference values used in D4 for cerium and the corresponding extrapolated value for the element. Its $P_{int}$ value was determined as average of the two neighbouring lanthanides praseodymium (Pr) and lanthanum (La).

Table S4: Atomic radii,[78] homoatomic $C_6$ and homoatomic $C_8$ dispersion coefficients from D4 of elements 1 – 43.

| **Number** | **Element** | **Radius [a.u.]** | **$C_6^{AA}$ [a.u.]** | **$C_8^{AA}$ [a.u.]** |
|---|---|---|---|---|
| 1 | H | 1.54 | 7.6 | 92.1 |
| 2 | He | 1.34 | 1.6 | 11.5 |
| 3 | Li | 2.20 | 1244.1 | 94049.3 |
| 4 | Be | 2.19 | 263.1 | 11722.3 |
| 5 | B | 2.05 | 108.2 | 4312.6 |
| 6 | C | 1.90 | 49.3 | 1425.4 |
| 7 | N | 1.79 | 25.4 | 559.4 |
| 8 | O | 1.71 | 15.6 | 314.2 |
| 9 | F | 1.63 | 9.7 | 166.5 |
| 10 | Ne | 1.56 | 6.3 | 93.1 |
| 11 | Na | 2.25 | 1705.6 | 221932.0 |
| 12 | Mg | 2.40 | 702.1 | 62861.9 |
| 13 | Al | 2.39 | 552.1 | 52916.2 |
| 14 | Si | 2.32 | 321.3 | 22981.7 |
| 15 | P | 2.23 | 192.8 | 10683.4 |
| 16 | S | 2.14 | 134.6 | 6594.6 |
| 17 | Cl | 2.06 | 92.7 | 3867.8 |
| 18 | Ar | 1.97 | 64.9 | 2312.2 |
| 19 | K | 2.34 | 5587.9 | 1066886.2 |
| 20 | Ca | 2.70 | 2454.7 | 368739.5 |
| 21 | Sc | 2.63 | 1583.8 | 207502.0 |
| 22 | Ti | 2.57 | 1412.3 | 167515.4 |
| 23 | V | 2.52 | 1154.6 | 127925.8 |
| 24 | Cr | 2.33 | 716.0 | 66081.3 |
| 25 | Mn | 2.42 | 827.5 | 83649.3 |
| 26 | Fe | 2.26 | 507.2 | 47443.5 |
| 27 | Co | 2.22 | 545.2 | 47937.1 |
| 28 | Ni | 2.19 | 589.5 | 49394.8 |
| 29 | Cu | 2.17 | 346.4 | 28377.3 |
| 30 | Zn | 2.22 | 346.6 | 27025.1 |
| 31 | Ga | 2.33 | 493.7 | 55499.4 |
| 32 | Ge | 2.34 | 367.7 | 33862.0 |
| 33 | As | 2.31 | 264.7 | 20389.7 |
| 34 | Se | 2.24 | 214.8 | 15282.3 |
| 35 | Br | 2.19 | 167.8 | 10612.7 |
| 36 | Kr | 2.12 | 130.9 | 7299.1 |
| 37 | Rb | 2.40 | 6914.8 | 1893779.1 |
| 38 | Sr | 2.79 | 3538.6 | 798707.8 |
| 39 | Y | 2.74 | 2460.8 | 469179.8 |
| 40 | Zr | 2.68 | 1885.7 | 312667.0 |
| 41 | Nb | 2.51 | 1522.2 | 198146.9 |
| 42 | Mo | 2.44 | 868.9 | 100052.6 |
| 43 | Tc | 2.41 | 1098.5 | 119233.6 |

Table S5: Atomic radii,[78] homoatomic $C_6$ and homoatomic $C_8$ dispersion coefficients from D4 of elements 44 – 86.

| **Number** | **Element** | **Radius [a.u.]** | **$C_6^{AA}$ [a.u.]** | **$C_8^{AA}$ [a.u.]** |
|---|---|---|---|---|
| 44 | Ru | 2.37 | 612.6 | 62171.7 |
| 45 | Rh | 2.33 | 729.4 | 70028.0 |
| 46 | Pd | 2.15 | 620.4 | 56845.0 |
| 47 | Ag | 2.25 | 436.7 | 38803.8 |
| 48 | Cd | 2.38 | 476.2 | 44529.3 |
| 49 | In | 2.46 | 775.6 | 114692.2 |
| 50 | Sn | 2.48 | 636.4 | 79880.7 |
| 51 | Sb | 2.46 | 497.3 | 53364.7 |
| 52 | Te | 2.42 | 428.4 | 43486.4 |
| 53 | I | 2.38 | 353.8 | 32495.2 |
| 54 | Xe | 2.32 | 291.4 | 24140.0 |
| 55 | Cs | 2.49 | 10848.2 | 3953688.4 |
| 56 | Ba | 2.93 | 6039.5 | 1869098.0 |
| 57 | La | 2.84 | 4173.1 | 1094852.7 |
| 58 | Ce | 2.82 | 393.8 | 97170.0 |
| 59 | Pr | 2.86 | 4621.1 | 1116042.3 |
| 60 | Nd | 2.84 | 4124.0 | 980196.1 |
| 61 | Pm | 2.83 | 3896.0 | 917478.6 |
| 62 | Sm | 2.80 | 3694.9 | 861802.0 |
| 63 | Eu | 2.80 | 3520.8 | 816687.9 |
| 64 | Gd | 2.77 | 1971.0 | 369001.9 |
| 65 | Tb | 2.76 | 3093.6 | 719661.8 |
| 66 | Dy | 2.75 | 2901.1 | 617674.3 |
| 67 | Ho | 2.73 | 2783.1 | 609333.0 |
| 68 | Er | 2.72 | 2657.4 | 572731.6 |
| 69 | Tm | 2.71 | 2543.6 | 544966.6 |
| 70 | Yb | 2.77 | 2494.8 | 537372.6 |
| 71 | Lu | 2.70 | 1678.4 | 309113.1 |
| 72 | Hf | 2.64 | 1481.6 | 299383.0 |
| 73 | Ta | 2.58 | 1190.3 | 212030.9 |
| 74 | W | 2.53 | 832.0 | 134019.0 |
| 75 | Re | 2.49 | 852.3 | 126678.4 |
| 76 | Os | 2.44 | 688.9 | 92491.2 |
| 77 | Ir | 2.33 | 573.3 | 63044.3 |
| 78 | Pt | 2.30 | 395.8 | 41158.7 |
| 79 | Au | 2.26 | 346.2 | 33822.4 |
| 80 | Hg | 2.29 | 365.2 | 36657.3 |
| 81 | Tl | 2.42 | 812.2 | 148160.0 |
| 82 | Pb | 2.49 | 750.4 | 118800.2 |
| 83 | Bi | 2.50 | 623.7 | 86056.7 |
| 84 | Po | 2.50 | 567.0 | 75879.3 |
| 85 | At | 2.47 | 486.5 | 59598.0 |
| 86 | Rn | 2.43 | 414.7 | 46226.8 |

Table S6 contains the valences, the atomic radii, homoatomic $C_6$ and homoatomic $C_8$ dispersion coefficients from D4 of all main group elements until radon in their respective hydrides. Table S7 contains the valences, the atomic radii, homoatomic $C_6$ and homoatomic $C_8$ dispersion coefficients from D4 of all main group elements until radon in their respective fluorides.

Table S6: Atomic radii, homoatomic $C_6$ and homoatomic $C_8$ dispersion coefficients from D4 of main group elements until Z = 86 in their respective hydrides with the given valence.

| **Number** | **Element** | **Valence** | **Radius [a.u.]** | **$C_6^{AA}$ [a.u.]** | **$C_8^{AA}$ [a.u.]** |
|---|---|---|---|---|---|
| 1 | H | 1 | 1.34 | 3.1 | 37.6 |
| 2 | He | 0 | 1.34 | 1.6 | 11.2 |
| 3 | Li | 1 | 0.99 | 41.1 | 3106.4 |
| 4 | Be | 2 | 1.73 | 30.6 | 1361.1 |
| 5 | B | 3 | 1.61 | 46.2 | 1840.1 |
| 6 | C | 4 | 1.90 | 31.0 | 893.2 |
| 7 | N | 3 | 1.83 | 41.9 | 923.0 |
| 8 | O | 2 | 1.72 | 24.7 | 499.6 |
| 9 | F | 1 | 1.59 | 11.8 | 200.9 |
| 10 | Ne | 0 | 1.55 | 6.3 | 92.9 |
| 11 | Na | 1 | 1.48 | 114.9 | 14944.2 |
| 12 | Mg | 2 | 1.78 | 86.3 | 7723.7 |
| 13 | Al | 3 | 1.76 | 148.9 | 14268.1 |
| 14 | Si | 4 | 2.05 | 159.9 | 11436.3 |
| 15 | P | 3 | 2.07 | 172.1 | 9535.2 |
| 16 | S | 2 | 2.00 | 148.5 | 7276.6 |
| 17 | Cl | 1 | 1.91 | 101.8 | 4248.9 |
| 18 | Ar | 0 | 1.97 | 64.9 | 2313.8 |
| 19 | K | 1 | 1.82 | 203.0 | 38744.8 |
| 20 | Ca | 2 | 1.69 | 225.9 | 33935.7 |
| 31 | Ga | 3 | 1.82 | 253.6 | 28512.0 |
| 32 | Ge | 4 | 2.09 | 189.8 | 17478.0 |
| 33 | As | 3 | 2.11 | 239.9 | 18481.9 |
| 34 | Se | 2 | 2.07 | 233.5 | 16610.8 |
| 35 | Br | 1 | 2.01 | 184.5 | 11665.0 |
| 36 | Kr | 0 | 2.12 | 130.9 | 7299.2 |
| 37 | Rb | 1 | 1.97 | 306.4 | 83917.0 |
| 38 | Sr | 2 | 1.83 | 271.0 | 61176.6 |
| 49 | In | 3 | 1.97 | 287.3 | 42488.8 |
| 50 | Sn | 4 | 2.20 | 335.9 | 42160.6 |
| 51 | Sb | 3 | 2.24 | 422.3 | 45324.1 |
| 52 | Te | 2 | 2.22 | 439.2 | 44582.1 |
| 53 | I | 1 | 2.17 | 380.5 | 34949.7 |
| 54 | Xe | 0 | 2.32 | 291.4 | 24141.9 |
| 55 | Cs | 1 | 2.15 | 416.8 | 151906.9 |
| 56 | Ba | 2 | 2.02 | 470.2 | 145528.5 |
| 81 | Tl | 3 | 2.04 | 363.7 | 66348.5 |
| 82 | Pb | 4 | 2.23 | 418.6 | 66261.0 |
| 83 | Bi | 3 | 2.26 | 519.6 | 71684.2 |
| 84 | Po | 2 | 2.23 | 568.0 | 76002.5 |
| 85 | At | 1 | 2.20 | 512.8 | 62822.7 |
| 86 | Rn | 0 | 2.43 | 414.7 | 46229.8 |

Table S7: Atomic radii, homoatomic $C_6$ and homoatomic $C_8$ dispersion coefficients from D4 of main group elements until Z = 86 in their respective fluorides with the given valence.

| **Number** | **Element** | **Valence** | **Radius [a.u.]** | **$C_6^{AA}$ [a.u.]** | **$C_8^{AA}$ [a.u.]** |
|---|---|---|---|---|---|
| 1 | H | 1 | 1.14 | 0.93 | 11.2 |
| 2 | He | 0 | 1.34 | 1.6 | 11.2 |
| 3 | Li | 1 | 1.01 | 73.1 | 5527.5 |
| 4 | Be | 2 | 1.62 | 38.9 | 1729.6 |
| 5 | B | 3 | 1.69 | 42.9 | 1708.2 |
| 6 | C | 4 | 1.88 | 20.9 | 605.2 |
| 7 | N | 3 | 1.73 | 19.1 | 421.1 |
| 8 | O | 2 | 1.62 | 14.0 | 283.6 |
| 9 | F | 1 | 1.51 | 9.4 | 160.7 |
| 10 | Ne | 0 | 1.55 | 6.3 | 92.9 |
| 11 | Na | 1 | 1.37 | 186.3 | 24231.2 |
| 12 | Mg | 2 | 1.50 | 150.6 | 13485.4 |
| 13 | Al | 3 | 1.69 | 201.8 | 19340.5 |
| 14 | Si | 4 | 1.98 | 197.2 | 14107.6 |
| 15 | P | 3 | 2.03 | 168.9 | 9359.6 |
| 16 | S | 2 | 1.95 | 128.5 | 6294.0 |
| 17 | Cl | 1 | 1.81 | 94.9 | 3961.7 |
| 18 | Ar | 0 | 1.97 | 64.9 | 2313.8 |
| 19 | K | 1 | 1.77 | 446.5 | 85246.2 |
| 20 | Ca | 2 | 1.62 | 553.2 | 83108.3 |
| 31 | Ga | 3 | 1.80 | 234.1 | 26307.0 |
| 32 | Ge | 4 | 1.98 | 213.9 | 19697.3 |
| 33 | As | 3 | 2.05 | 237.2 | 18269.8 |
| 34 | Se | 2 | 1.97 | 216.2 | 15380.8 |
| 35 | Br | 1 | 1.90 | 176.5 | 11160.3 |
| 36 | Kr | 0 | 2.12 | 130.9 | 7299.2 |
| 37 | Rb | 1 | 1.94 | 590.8 | 161809.1 |
| 38 | Sr | 2 | 1.81 | 684.7 | 154539.2 |
| 49 | In | 3 | 1.93 | 348.9 | 51598.6 |
| 50 | Sn | 4 | 2.04 | 348.1 | 43695.4 |
| 51 | Sb | 3 | 2.17 | 398.8 | 42792.2 |
| 52 | Te | 2 | 2.12 | 400.9 | 40694.9 |
| 53 | I | 1 | 2.06 | 358.5 | 32929.9 |
| 54 | Xe | 0 | 2.32 | 291.4 | 24141.9 |
| 55 | Cs | 1 | 2.15 | 924.5 | 336921.0 |
| 56 | Ba | 2 | 2.04 | 1249.2 | 386586.1 |
| 81 | Tl | 3 | 2.02 | 432.9 | 78969.0 |
| 82 | Pb | 4 | 2.05 | 453.9 | 71869.9 |
| 83 | Bi | 3 | 2.15 | 517.0 | 71323.2 |
| 84 | Po | 2 | 2.08 | 545.7 | 73020.5 |
| 85 | At | 1 | 2.06 | 497.0 | 60894.5 |
| 86 | Rn | 0 | 2.43 | 414.7 | 46229.8 |

## 3.2 Case Studies

Table S8 contains the training set parameters and target values of the Pd-catalyzed enantioselective 1,1-diarylation of benzyl acrylates. Table S9 contains the corresponding validation set. The $NBO_{C1}$ parameters and the target values were taken from literature.[79]

Table S8: Training set parameters and target values of the Pd-catalyzed enantioselective 1,1-diarylation of benzyl acrylates.

| $\mathbf{P_{int}}$ [$\mathbf{kcal^{0.5}\ mol^{-0.5}}$] | $\mathbf{A_{rel}}$ | $\mathbf{P_{int}\ A_{rel}}$ [$\mathbf{kcal^{0.5}\ mol^{-0.5}}$] | $\mathbf{NBO_{C1}}$ [a.u.] | $\mathbf{\Delta\Delta G^{\ddagger}}$ [$\mathbf{kcal\ mol^{-1}}$] |
|---|---|---|---|---|
| 15.3 | 2.52 | 38.6 | -0.060 | 1.13 |
| 15.4 | 3.19 | 49.1 | -0.025 | 1.63 |
| 16.7 | 3.26 | 54.4 | -0.116 | 0.43 |
| 14.9 | 2.85 | 42.5 | -0.214 | 0.62 |
| 15.8 | 3.80 | 60.0 | -0.080 | 0.92 |
| 15.9 | 3.48 | 55.3 | -0.041 | 1.24 |
| 15.8 | 3.24 | 51.2 | -0.032 | 1.45 |
| 15.1 | 2.76 | 41.7 | -0.012 | 1.49 |
| 16.9 | 3.57 | 60.3 | -0.023 | 1.51 |
| 16.1 | 3.95 | 63.6 | -0.029 | 1.63 |
| 16.7 | 4.60 | 76.8 | -0.043 | 1.63 |
| 17.1 | 3.40 | 58.1 | -0.020 | 2.30 |

Table S9: Validation set parameters and target values of the Pd-catalyzed enantioselective 1,1-diarylation of benzyl acrylates.

| $\mathbf{P_{int}}$ [$\mathbf{kcal^{0.5}\ mol^{-0.5}}$] | $\mathbf{A_{rel}}$ | $\mathbf{P_{int}\ A_{rel}}$ [$\mathbf{kcal^{0.5}\ mol^{-0.5}}$] | $\mathbf{NBO_{C1}}$ [a.u.] | $\mathbf{\Delta\Delta G^{\ddagger}}$ [$\mathbf{kcal\ mol^{-1}}$] |
|---|---|---|---|---|
| 15.6 | 3.21 | 50.1 | -0.118 | 0.90 |
| 15.6 | 3.00 | 46.8 | -0.049 | 1.37 |
| 17.1 | 3.64 | 62.2 | -0.051 | 1.41 |
| 15.9 | 3.13 | 49.8 | -0.051 | 1.88 |
| 15.9 | 4.12 | 65.5 | -0.043 | 1.88 |
| 18.2 | 3.73 | 67.9 | -0.025 | 2.30 |

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benchmark/selenophene.xyz

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1.12581147962624     -0.01911171715478
  C   0.94853771919762      0.68627084009502
    -0.01452711772932
  C   1.11554458930666     -0.67238114624237
    -0.00600215662240
  Se  -0.52899843983656
-1.56122396665353     -0.00305962326907
  H   -2.42390306010341
0.21378546973274     -0.01632596916941
  H   -0.69007772451438
2.17995114710912     -0.02588439542380
  H   1.79255316884028      1.37698907752955
    -0.01751142026813
  H   2.04652063858870     -1.23207163421864
    -0.00124866111343
```

benchmark/benzene_dimer.xyz

```
24
benzene t dimer
C      1.391500000000    -0.000000000000
2.495750000000
H      2.471500000000    -0.000000000000
```

2.495750000000
C 0.695750000000 1.205074349366
2.495750000000
H 1.235750000000 2.140381785453
2.495750000000
C 0.695750000000 -1.205074349366
2.495750000000
H 1.235750000000 -2.140381785453
2.495750000000
C -0.695750000000 1.205074349366
2.495750000000
H -1.235750000000 2.140381785453
2.495750000000
C -0.695750000000 -1.205074349366
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2.495750000000
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2.495750000000
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-1.104250000000
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-1.800000000000
H -0.000000000000 -2.140381785453
-1.260000000000
H 0.000000000000 0.000000000000
-0.024250000000
C -0.000000000000 -1.205074349366
-3.191500000000

```
H      -0.000000000000    -2.140381785453
-3.731500000000
C      -0.000000000000     0.000000000000
-3.887250000000
H      -0.000000000000     0.000000000000
-4.967250000000
C      -0.000000000000     1.205074349366
-3.191500000000
H       0.000000000000     2.140381785453
-3.731500000000
C       0.000000000000     1.205074349366
-1.800000000000
H       0.000000000000     2.140381785453
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benchmark/ethane.xyz

8
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     0.01295878534956
  H   0.65273636633025      1.08570461282665
     0.20272122847174
  H   0.65273425230549     -0.58751898449587
     0.78922457511641
  H   0.65272514750968     -0.25883339573031
    -0.95307830661943
  H   2.98503485983221      0.41840586972115
```

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  H   2.98502572528557      0.74709151118844
    -0.76331205418906
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    -0.17680876341588

benchmark/furan.xyz

9
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  C   -0.37753893745183
1.14948916835559     -0.00012600250167
  C   0.98262087230777      0.69759316806982
     0.00064936356023
  C   0.93074878861096     -0.66601370908205
    -0.00521418795469
  O   -0.36829818189328
-1.09560728145426     -0.00951602219699
  H   -2.22212052900797
-0.14810959596672     -0.00909506607973
  H   -0.73097157395478
2.17565795282955      0.00348088903763
  H   1.87985798013853      1.30824439533099
     0.00496180474198
  H   1.68394647943887     -1.44586426958550
    -0.00704313666253

benchmark/tellurophene.xyz
```

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9
Coordinates from ORCA-job
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     0.01364044416861
  C   0.71701929107721     -0.94042954306621
     0.00413446410744
  C   -0.7155937945288
-0.94178976570971      0.00414778447772
  C   -1.35534157843301
0.26614249469651      0.01366482944950
  Te  -0.00191355975180
1.82595115414866      0.02598436974276
  H   2.42924831784412      0.43222691927662
     0.01489662608321
  H   1.28116225188532     -1.87619612212847
    -0.00326305348939
  H   -1.2779597216921
-1.87862541141793     -0.00323837399479
  H   -2.43042490248988
0.42761546945220      0.01494290945495

benchmark/perfluoroethane.xyz

8
Coordinates from ORCA-job
/scratch/84771885.tmpdir/opt1_pbe_tzvp
  F   1.73287617010030     -1.00148501393146
     0.82172879869054
  C   2.34443170766124     -0.08097276076943
```

```
    0.0554776011302 9
  F   1.4684841114019 9     0.8954624624396 3
   -0.2409882698292 0
  F   3.3743077190963 6     0.4464974567050 5
    0.7407388805004 9
  C   2.8655276717471 7    -0.7452557978839 2
   -1.2599845292353 0
  F   1.8356312109599 1    -1.2726932346705 0
   -1.9452530950705 6
  F   3.4771026959585 5     0.1752476621730 9
   -2.0262299008538 5
  F   3.7414469540744 8    -1.7217117050624 7
   -0.9635297133324 1

benchmark/thiophene.xyz

9
Coordinates from ORCA-job
/scratch/83715721.tmpdir/opt1_pbe_tzvp
  C   -1.1924454376801 9
0.0250698334717 1     0.0020208459727 2
  C   -0.4715090297733 8
1.1960383896578 4     0.0005701114720 1
  S   1.2205298818164 0     0.8897941561537 2
   -0.0017320013055 3
  C   0.9790074877922 1    -0.8126714907917 7
   -0.0008841243930 0
  C   -0.3592803574782 7
-1.1287173751815 5     0.0011846176585 2
  H   -2.2811668290907 6
-0.0070904078992 4     0.0036090044222 7
```

```
  H   -0.84040753960913
2.21767295629929      0.00075640095058
  H   1.83278096045286     -1.48415827353008
    -0.00192714571810
  H   -0.73221913642974
-2.15207778817990      0.00205229094053

benchmark/pyrrole.xyz

10
Coordinates from ORCA-job
/scratch/84795567.tmpdir/opt1_pbe_tzvp
  C   -1.17985459125872
0.01042501570445      0.00013924161948
  C   -0.37744924233702
1.13681901727390      0.00040592875762
  C   0.97650019843311      0.69663504349282
    0.00015951520912
  C   0.96310094340141     -0.68626300006728
    -0.00022700556713
  N   -0.35208174306223
-1.08752937089968     -0.00023902409811
  H   -2.25921270751020
-0.09836933168157      0.00019319286226
  H   -0.72832305697630
2.16420013619483      0.00073285774632
  H   1.86445318895881      1.32126487815045
    0.00026215404584
  H   1.77212975338411     -1.40898271111676
    -0.00049727628105
  H   -0.66490274303294
```

```
-2.0497196770511 8     -0.0004895842943 7

benchmark/ethene.xyz

6
Coordinates from ORCA-job
/scratch/84734644.tmpdir/opt1_pbe_tzvp
  C   1.0047663769029 8     -0.0462166569324 1
    -0.0882166894225 6
  C   2.3374969573600 6     -0.0462166583409 0
    -0.0882166909644 5
  H   0.4305368972014 0      0.7958186179104 0
     0.3036019687159 9
  H   0.4305368916918 7     -0.8882519578829 9
    -0.4800352779339 3
  H   2.9117264317539 2      0.7958186174367 4
     0.3036019718318 1
  H   2.9117264450897 7     -0.8882519621908 2
    -0.4800352822268 7

benchmark/ethyne.xyz

4
Coordinates from ORCA-job
/scratch/84734645.tmpdir/opt1_pbe_tzvp
  C   1.0748478922310 4      0.0936499947708 8
     0.0226800000594 7
  C   2.2825021144807 6      0.0936499880266 2
     0.0226800045379 6
  H   0.0038531412808 8      0.0936500074774 2
     0.0226799984467 5
```

```
  H   3.3534968520073      0.0936500097250
    0.0226799969558

benchmark/pd_imine.xyz

17
Coordinates from ORCA-job
/scratch/84734775.tmpdir/opt1_pbe_tzvp
  C   -2.8575873413783
3.6878809701455     -2.3523189182897
  C   -4.0646825067362
3.0906852192328     -2.5742571948787
  C   -4.0095995489057
1.7393920816434     -3.0737702114276
  N   -2.8361280475837
1.2105803927347     -3.2686638394556
  Pd  -1.2703018521573
2.5940498063779     -2.7559522263159
  C   0.0166767588680      3.9905801332697
    -2.2337642017140
  C   1.3354420553055      3.6594988374821
    -2.3528775878105
  C   1.6034844576203      2.3316453355524
    -2.8464690851326
  N   0.5854505194129      1.5724106107391
    -3.1321884065136
  H   -2.8313627781220
4.7166732757000     -1.9719978377477
  H   -5.0332201781194
3.5684964716285     -2.3984594015130
  H   -4.9298120404248
```

```
1.1743417968259     -3.28296923412259
  H   2.16594375988437      4.32634027048808
    -2.10204732365863
  H   2.63505781840746      1.97298109886697
    -2.97699091924918
  H   0.82089912484169      0.64109430526496
    -3.47829123736740
  H   -0.2537853946487 9
4.98742912312155     -1.86366271754737
  H   -2.84411674926388
0.25274175992587     -3.62232482925549

benchmark/benzene.xyz

12
Coordinates from ORCA-job
/scratch/84795522.tmpdir/opt1_pbe_tzvp
  C   -0.76344466897431
1.18092155593116     -0.00461321000917
  C   0.63192060803559      1.25589372133713
    -0.00715444022441
  C   1.39451109351131      0.08494564863424
    -0.00892014988196
  C   0.76174458787796     -1.16094159148464
    -0.00814512145763
  C   -0.6336205965407 0
-1.23591368560157     -0.00560386779299
  C   -1.3962110715585 1
-0.06496572616803     -0.00383817296032
  H   -1.35919207414099
2.09567656466894     -0.00323609369678
```

```
  H   1.12626151103198      2.22919808930830
    -0.00776134301813
  H   2.48458711383869      0.14346637862240
    -0.01090460614265
  H   1.35749193461832     -2.07569654716190
    -0.00952226898755
  H   -1.1279614328340
-2.2092179188814     -0.00499700481082
  H   -2.4862870048653
-0.1234864892045     -0.00185372101757

benchmark/cu_nhc.xyz

10
Coordinates from ORCA-job
/scratch/84734515.tmpdir/opt1_pbe_tzvp
  Cu  0.97472137283189      0.10560346832212
    -0.08083094263691
  C   2.84864795626788      0.06686892100022
    -0.07148388779191
  N   3.70820232614067      1.11628703918554
    -0.06666442878316
  C   5.02675230345917      0.70399243643263
    -0.06028898931420
  C   4.99861526396798     -0.65959299648349
    -0.06111537499657
  N   3.66416858833244     -1.01713110395115
    -0.06795788410950
  H   3.41157207920293      2.08761677545219
    -0.06765845525128
  H   5.85847237454639      1.39845742498920
```

```
    -0.0557782425824
  H   5.80095215537597     -1.38781295803733
    -0.0574703901543
  H   3.32767557987469     -1.9753790069093
    -0.0701817384279

case_studies/cuh_hydroamination/2.xyz

  42
        -52.64199292
 H          -0.2096210244       -5.7763445003
       0.4915882486
 C          -0.1658200763       -4.7331243562
       0.3905793282
 C          -0.1149724488       -3.5393657350
       0.2734707906
 C          -0.0558196166       -2.1312376306
       0.1399468879
 C           1.1736794918       -1.4893786582
       0.0256351945
 C           1.2546328937       -0.1086743514
      -0.0226533549
 C           0.0565236507        0.6291967653
       0.0745335132
 C          -1.1955460174        0.0015699587
      -0.0187563501
 C          -1.2223788908       -1.3858124527
       0.0634103416
 H          -2.1618461789       -1.9155146105
       0.0745099725
 C          -2.5316760710        0.7020154438
```

-0.2792359596
C -2.4140748466 2.1784742043
-0.6743195456
H -1.6758784646 2.3074076456
-1.4612952938
H -3.3770958072 2.5231565476
-1.0486952314
H -2.1440944716 2.8157681143
0.1597190847
C -3.1993003170 -0.0007861695
-1.4773207129
H -2.5331260719 0.0115926557
-2.3373238797
H -3.4594886221 -1.0322718360
-1.2613639244
H -4.1157690906 0.5208336292
-1.7452304515
C -3.4468939795 0.5730278109
0.9461109448
H -3.0176282273 1.0733816679
1.8121185571
H -3.6066527986 -0.4704827302
1.2065784769
H -4.4133508488 1.0268977327
0.7366356695
O 0.1465540429 2.0012572252
0.2851041939
C -0.0970379220 2.3540578963
1.6303199593
H -1.1079883916 2.0835665888
1.9500411771

H 0.0245375456 3.4351674445 1.6905013260
H 0.6128414701 1.8680113469 2.3083879016
C 2.5953183994 0.5838832482 -0.2617068478
C 3.7188160137 -0.4213705959 -0.5441121150
H 3.9357825406 -1.0314530027 0.3300422430
H 4.6249142143 0.1234773013 -0.8021663674
H 3.4697039300 -1.0685238529 -1.3819322625
C 3.0291767111 1.4333019605 0.9405500551
H 2.4285562870 2.3321463931 1.0191759301
H 2.9480322585 0.8613836139 1.8635260535
H 4.0674563844 1.7360638563 0.8187544345
C 2.4527998938 1.4790219753 -1.5018884674
H 2.1873833074 0.8779146752 -2.3696169702
H 3.3942562845 1.9848834265 -1.7062056103
H 1.6818740895 2.2277274040 -1.3502091682
H 2.0581642161 -2.1025258011

```
      -0.0026100435

case_studies/cuh_hydroamination/5.xyz

  38
        -45.42976707
 H           0.0011564569        5.5736382007
      -0.0000801411
 C           0.0010715455        4.5245796007
      -0.0000877210
 C           0.0004335439        3.3240806707
       0.0000420890
 C           0.0001789920        1.9073077707
       0.0001153190
 C           1.2100278711        1.2179561691
       0.0000533193
 C           1.2222857992       -0.1677118609
       0.0001342894
 C          -0.0001405616       -0.8320437393
       0.0002015291
 C          -1.2223997307       -0.1674218977
       0.0002611487
 C          -1.2098231789        1.2182574323
       0.0002296587
 H          -2.1211725781        1.7935109035
       0.0002729085
 C          -2.5094612118       -0.9791745659
      -0.0000090716
 C          -2.5465283533       -1.8615765559
       1.2556671084
 H          -2.4945686027       -1.2442646059
```

```
      2.1502773884
H          -3.4713812241       -2.4341062546
      1.2844472382
H          -1.7147595343       -2.5603985270
      1.2763446787
C          -2.5471737627       -1.8589032659
     -1.2575412916
H          -2.4957304516       -1.2396635860
     -2.1508200616
H          -3.4719908334       -2.4314602447
     -1.2870878718
H          -1.7152929936       -2.5575249270
     -1.2800790113
C          -3.7611649807       -0.0974397343
      0.0013455181
H          -4.6485716715       -0.7275304231
      0.0012905279
H          -3.7973167096        0.5327378258
     -0.8843430419
H          -3.7963256600        0.5313026958
      0.8881034281
H          -0.0002598431       -1.9107243393
      0.0001590491
C           2.5091568882       -0.9797648727
     -0.0000023503
C           2.5462605667       -1.8613236527
      1.2562756398
H           2.4942426773       -1.2433996226
      2.1504464197
H           1.7145197557       -2.5601595816
      1.2773697795
```

```
 H           3.4711483959       -2.4337801939
      1.2854701900
 C           3.7610527593       -0.0983098243
      0.0004538400
 H           3.7966110000        0.5310083356
      0.8867931400
 H           4.6483202885       -0.7285844055
      0.0005661303
 H           3.7970610404        0.5312977356
     -0.8856601700
 C           2.5464222373       -1.8603812427
     -1.2569406002
 H           2.4949882184       -1.2417375627
     -2.1506467703
 H           3.4710896966       -2.4331847940
     -1.2862236500
 H           1.7143852964       -2.5588412016
     -1.2788837705
 H           2.1214826919        1.7930386879
     -0.0000809904
```

case_studies/cuh_hydroamination/ts6.xyz

```
175
symmetry c1
C       -1.054280000      1.669970000
-3.138280000
C       -0.834940000      0.378140000
-3.710940000
H       -0.244350000      2.392440000
-3.182800000
```

H -1.714480000 -0.111640000 -4.127660000
H -2.057480000 2.087290000 -3.161740000
C 0.442620000 0.105510000 -4.486630000
H 1.312770000 0.512340000 -3.960480000
H 0.610260000 -0.965060000 -4.644440000
H 0.385760000 0.600340000 -5.466230000
H -0.646940000 -0.878490000 -2.651800000
Cu -0.861560000 0.309420000 -1.547610000
P 0.875330000 0.362890000 -0.110760000
C 0.412720000 1.047430000 1.546980000
C 2.324390000 1.391860000 -0.647090000
C 1.669230000 -1.262010000 0.308590000
C -0.569330000 0.366400000 2.337710000
C 0.945760000 2.266880000 1.986820000
C 3.645670000 0.931660000 -0.672360000
C 2.048380000 2.681470000

-1.126060000
C 1.382350000 -2.350580000
-0.520260000
C 2.545590000 -1.428750000
1.387950000
C -0.894810000 0.983720000
3.537550000
C -1.166550000 -0.985960000
2.082440000
C 0.570200000 2.873780000
3.197090000
H 1.687420000 2.775810000
1.384560000
C 4.675510000 1.746080000
-1.152180000
H 3.889070000 -0.061500000
-0.322360000
C 3.081660000 3.509980000
-1.571380000
H 1.019790000 3.021430000
-1.150710000
C 1.986920000 -3.590390000
-0.288590000
H 0.675270000 -2.204720000
-1.332600000
C 3.168520000 -2.660780000
1.605250000
H 2.751610000 -0.601300000
2.057170000
C -0.356160000 2.197550000
3.958760000

C -0.790380000 -2.001030000 2.950630000
C -2.167640000 -1.336990000 1.117600000
H 1.000710000 3.815280000 3.519430000
C 4.399600000 3.045950000 -1.582030000
C 2.894410000 -3.741520000 0.760600000
C -1.308150000 -3.293480000 2.906490000
C -2.682980000 -2.639790000 1.095270000
P -2.659260000 -0.135270000 -0.208350000
C -2.265210000 -3.647690000 1.982390000
H -3.439480000 -2.890600000 0.361270000
C -4.032320000 -0.967790000 -1.127640000
C -3.461220000 1.247610000 0.710260000
H -2.675450000 -4.650550000 1.939560000
C -5.384620000 -0.777530000 -0.852400000
C -3.680190000 -1.832440000 -2.175740000
C -3.150400000 2.551960000

0.320310000
C -4.314910000 1.057470000
1.799340000
C -6.403430000 -1.364070000
-1.624610000
H -5.661600000 -0.146660000
-0.017240000
C -4.636000000 -2.431920000
-3.000490000
H -2.625910000 -2.010370000
-2.349980000
C -3.716680000 3.670470000
0.943750000
H -2.431350000 2.676310000
-0.480110000
C -4.937040000 2.125120000
2.465150000
H -4.480250000 0.046750000
2.150100000
C -5.996400000 -2.091850000
-2.765330000
C -4.679250000 3.429560000
1.960690000
C 4.195020000 -2.755500000
2.722390000
C 1.642240000 -4.808830000
-1.131590000
C -4.207060000 -3.473500000
-4.067050000
C -7.860780000 -1.191040000
-1.108440000

C -3.233840000 5.092540000
0.553680000
C -5.821000000 1.806290000
3.704880000
C 6.095370000 1.195920000
-1.137170000
C 2.817290000 4.944410000
-2.004820000
F 3.946680000 5.472890000
-2.605740000
F 6.071560000 -0.165570000
-0.889300000
F 3.929540000 -1.797030000
3.686120000
F 2.501500000 -5.851770000
-0.827610000
H 5.187950000 3.695740000
-1.933790000
H 3.369770000 -4.700070000
0.914280000
C 1.699000000 5.070460000
-3.073010000
C 2.553360000 5.853930000
-0.776490000
C 6.818170000 1.334260000
-2.501750000
C 6.919070000 1.802150000
0.027460000
C 1.825160000 -4.572600000
-2.654320000
C 0.226630000 -5.343010000

-0.788530000
C 5.613790000 -2.418460000
2.188900000
C 4.184680000 -4.105250000
3.485960000
F 0.482530000 4.862580000
-2.527880000
F 1.704120000 6.287320000
-3.627700000
F 1.887220000 4.165160000
-4.043730000
F 2.315400000 7.120590000
-1.141540000
F 1.497960000 5.414830000
-0.065100000
F 3.632040000 5.840670000
0.020990000
F 7.960830000 0.638370000
-2.511120000
F 7.111470000 2.622470000
-2.770400000
F 6.033320000 0.865610000
-3.482190000
F 8.151660000 1.281290000
0.083800000
F 7.029120000 3.135930000
-0.106140000
F 6.300260000 1.541530000
1.189260000
F 3.020350000 -4.009590000
-2.886550000

F 0.869380000 -3.759370000 -3.142210000
F 1.770500000 -5.729860000 -3.324920000
F -0.063120000 -6.448310000 -1.489030000
F -0.717050000 -4.419710000 -1.048350000
F 0.171200000 -5.646770000 0.516980000
F 6.538080000 -2.500980000 3.156360000
F 5.621380000 -1.163120000 1.711020000
F 5.958500000 -3.254730000 1.197540000
F 2.921880000 -4.464640000 3.786340000
F 4.868860000 -4.011940000 4.629800000
F 4.729760000 -5.091180000 2.747240000
O -0.888370000 2.550220000 5.171520000
O -1.780400000 0.531570000 4.489180000
C -1.612730000 1.399170000 5.614510000
H -1.035580000 0.880030000 6.392950000
H -2.592670000 1.706000000

5.986380000
O 0.152960000 -1.925390000
3.949480000
O -0.711240000 -4.066660000
3.870250000
C 0.032800000 -3.150090000
4.679710000
H 1.026490000 -3.554850000
4.870680000
H -0.512950000 -2.964990000
5.616410000
C -5.648880000 2.852260000
4.833250000
H -4.594880000 2.931610000
5.126400000
H -5.978460000 3.850730000
4.551560000
H -6.220400000 2.534840000
5.713510000
C -7.311910000 1.687310000
3.302290000
H -7.920070000 1.439230000
4.181380000
H -7.712600000 2.605750000
2.870680000
H -7.449890000 0.887910000
2.565510000
C -5.426690000 0.441420000
4.327430000
H -4.351290000 0.375660000
4.520040000

H -5.957730000 0.315790000
5.277810000
H -5.708740000 -0.407580000
3.696080000
C -2.036920000 5.036970000
-0.422420000
H -1.191340000 4.482200000
-0.002680000
H -2.297930000 4.588290000
-1.386920000
H -1.692560000 6.058000000
-0.620650000
C -4.348050000 5.898900000
-0.153190000
H -4.732170000 5.355740000
-1.024850000
H -5.183790000 6.120720000
0.510190000
H -3.946090000 6.856290000
-0.507070000
C -2.742430000 5.850980000
1.812110000
H -2.381290000 6.846950000
1.526690000
H -3.534310000 5.968330000
2.552680000
H -1.909040000 5.314730000
2.281630000
C -8.924710000 -2.088150000
-1.782710000
H -9.153880000 -1.795790000

-2.807750000
H -8.625140000 -3.139640000
-1.790630000
H -9.855940000 -2.006190000
-1.208830000
C -8.296560000 0.287780000
-1.240180000
H -8.311530000 0.610100000
-2.287520000
H -9.306310000 0.424760000
-0.833290000
H -7.621200000 0.958520000
-0.697820000
C -7.888990000 -1.586150000
0.394330000
H -8.906590000 -1.474250000
0.786580000
H -7.588790000 -2.631800000
0.527550000
H -7.230780000 -0.968410000
1.011040000
C -2.694020000 -3.774050000
-3.988010000
H -2.079650000 -2.899230000
-4.228690000
H -2.391880000 -4.139070000
-3.001570000
H -2.449820000 -4.555090000
-4.716870000
C -4.496860000 -3.001020000
-5.511860000

H -4.074780000 -2.005840000 -5.697070000
H -4.034720000 -3.694750000 -6.224770000
H -5.565420000 -2.975020000 -5.727450000
C -4.953870000 -4.804990000 -3.803200000
H -4.647950000 -5.557600000 -4.540690000
H -4.710820000 -5.194620000 -2.807570000
H -6.036100000 -4.677110000 -3.871400000
O -6.935950000 -2.517990000 -3.691640000
O -5.291800000 4.539770000 2.522230000
C -7.353950000 -1.495960000 -4.597980000
H -6.501660000 -1.071980000 -5.140980000
H -8.036670000 -1.972870000 -5.305980000
H -7.878840000 -0.684070000 -4.082020000
C -6.627560000 4.855470000 2.133680000
H -7.333210000 4.588930000 2.928190000
H -6.683280000 5.937230000

```
1.977400000
H       -6.911390000      4.344070000
1.207880000

case_studies/cuh_hydroamination/6.xyz

  20
        -26.43951495
 H           4.7312167982       -0.0050170225
      0.0007581817
 C           3.6821635629       -0.0043608995
      0.0003531155
 C           2.4816877512       -0.0028954373
      0.0003559571
 C           1.0653983543       -0.0013709163
      0.0000748819
 C           0.3666075882       -1.2072161032
      0.0067322774
 C          -1.0184322583       -1.2123046824
      0.0063291833
 C          -1.6959224174        0.0015212858
     -0.0018024573
 C          -1.0169537053        1.2129027841
     -0.0092219379
 C           0.3693323280        1.2048207896
     -0.0076095101
 H           0.9198686861        2.1347504945
     -0.0126407424
 C          -1.7725092990        2.5077131742
      0.0059836980
 H          -1.1815814701        3.3077107854
```

```
      -0.4338559013
 H         -2.7083297643         2.4170248351
      -0.5412203974
 H         -2.0094215181         2.7879019679
       1.0331384206
 H         -2.7773482219         0.0010891824
      -0.0028876344
 C         -1.7846487765        -2.5009178126
      -0.0028955040
 H         -2.2262636811        -2.6666781072
      -0.9858909712
 H         -2.5936584693        -2.4719112159
       0.7248989371
 H         -1.1353854410        -3.3422101801
       0.2264586863
 H          0.9164904498        -2.1375421796
       0.0115036071
```

case_studies/cuh_hydroamination/ts4.xyz

```
107
symmetry c1
C        -0.076300000     -0.425700000
-3.881410000
C        -0.337870000      0.940060000
-3.540250000
H        -0.943130000     -1.020420000
-4.167360000
H         0.429710000      1.675100000
-3.769270000
C         1.183810000     -0.783940000
```

-4.649520000
H 2.055380000 -0.258090000
-4.245830000
H 1.389760000 -1.858880000
-4.626910000
H -1.360400000 1.300700000
-3.619510000
H 1.064720000 -0.473730000
-5.696610000
H 0.198070000 -1.456760000
-2.615900000
Cu -0.007200000 -0.087960000
-1.734950000
P 1.727780000 0.295240000
-0.326880000
C 1.214170000 1.224390000
1.189190000
C 3.102480000 1.315040000
-1.041470000
C 2.626140000 -1.181290000
0.343250000
C 0.249570000 0.657720000
2.084520000
C 1.681940000 2.528760000
1.399370000
C 4.463970000 1.093520000
-0.797260000
C 2.735810000 2.335690000
-1.929940000
C 2.581520000 -2.363240000
-0.400660000

```
C         3.341870000     -1.159960000
1.551330000
C        -0.145330000      1.477690000
3.131920000
C        -0.285570000     -0.742950000
2.084940000
C         1.249620000      3.334070000
2.466970000
H         2.412310000      2.948010000
0.718290000
C         5.432330000      1.876230000
-1.430930000
H         4.782900000      0.312410000
-0.117130000
C         3.707110000      3.121510000
-2.552370000
H         1.684900000      2.498920000
-2.147200000
C         3.258540000     -3.504890000
0.042370000
H         1.992510000     -2.395280000
-1.314910000
C         4.009840000     -2.302550000
1.988660000
H         3.368230000     -0.260430000
2.156280000
C         0.327840000      2.774780000
3.324040000
O        -1.060730000      1.179650000
4.110580000
C         0.123860000     -1.577980000
```

3.114140000
C -1.279490000 -1.287130000
1.208950000
H 1.626490000 4.340700000
2.608890000
C 5.061130000 2.894550000
-2.309420000
C 3.975760000 -3.480290000
1.233890000
O -0.266650000 3.329720000
4.423220000
C -1.001810000 2.266970000
5.044300000
C -0.362760000 -2.870920000
3.302150000
O 1.062120000 -1.300530000
4.076030000
C -1.761810000 -2.586280000
1.414450000
P -1.768150000 -0.350510000
-0.305150000
H -2.013560000 2.604950000
5.266280000
H -0.473910000 1.940650000
5.950510000
C -1.314760000 -3.407910000
2.463720000
O 0.249180000 -3.447060000
4.380960000
C 1.042230000 -2.414090000
4.980840000

H -2.509910000 -2.987910000 0.741370000
C -3.165110000 -1.326910000 -1.035300000
C -2.631040000 1.155920000 0.339980000
H -1.701400000 -4.410860000 2.605610000
H 0.581520000 -2.105470000 5.928470000
H 2.060850000 -2.774450000 5.127640000
C -4.513890000 -1.148300000 -0.697200000
C -2.838980000 -2.254070000 -2.033110000
C -2.589410000 2.304880000 -0.456370000
C -3.318460000 1.196620000 1.562770000
C -5.508450000 -1.881400000 -1.347280000
H -4.800860000 -0.438320000 0.069890000
C -3.838290000 -2.983990000 -2.680620000
H -1.796200000 -2.392480000 -2.307500000
C -3.240670000 3.473290000 -0.049210000
H -2.035970000 2.285770000

-1.391680000
C -3.965380000 2.365850000
1.962790000
H -3.343310000 0.324090000
2.206330000
C -5.177570000 -2.801520000
-2.344320000
C -3.932620000 3.509010000
1.158020000
C 4.765730000 -2.309300000
3.290720000
C 3.193790000 -4.753150000
-0.801070000
C -3.428160000 -3.950650000
-3.762010000
C -6.957540000 -1.628120000
-1.016010000
C -3.133930000 4.704750000
-0.912830000
C -4.684580000 2.437470000
3.283760000
C 6.892740000 1.574070000
-1.207040000
C 3.263680000 4.231130000
-3.471980000
F -4.004460000 3.212340000
4.171970000
F -5.906120000 2.994090000
3.154070000
F -4.840070000 1.227040000
3.852480000

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F        -4.040200000      5.643270000
-0.569340000
F        -3.320840000      4.408960000
-2.216110000
F        -1.910020000      5.268830000
-0.808010000
F        -7.470880000     -0.637150000
-1.777650000
F        -7.116460000     -1.259170000
0.273580000
F        -7.716390000     -2.724440000
-1.225870000
F        -2.745820000     -3.317600000
-4.744450000
F        -4.488100000     -4.559990000
-4.330140000
F        -2.613420000     -4.912700000
-3.278590000
F         2.773230000      5.279770000
-2.774780000
F         4.277310000      4.691890000
-4.232850000
F         2.281090000      3.817090000
-4.302120000
F         7.663130000      2.666690000
-1.391470000
F         7.336010000      0.624950000
-2.060150000
F         7.119000000      1.118060000
0.044190000
F         6.037710000     -2.726220000
```

3.123260000
F 4.198400000 -3.166880000
4.182600000
F 4.802200000 -1.096630000
3.873730000
F 3.777050000 -5.807500000
-0.193840000
F 3.812890000 -4.573990000
-1.988110000
F 1.915250000 -5.092540000
-1.072110000
H -4.442580000 4.413640000
1.469490000
H -5.952340000 -3.365450000
-2.849610000
H 5.815160000 3.498270000
-2.799840000
H 4.495190000 -4.367280000
1.578570000

case_studies/cuh_hydroamination/7.xyz

14
-20.09784636
H -4.2294394689 0.0000535378
0.0001142219
C -3.1803609889 0.0000148485
0.0000613312
C -1.9799030489 -0.0000283707
-0.0000214895
C -0.5637012689 -0.0000498597

-0.0000465804
C 0.1374945119 -1.2056186393
-0.0000240816
C 1.5192015619 -1.1999444983
0.0000025976
C 2.2124037611 0.0000496722
0.0000461679
C 1.5191124802 1.2000040017
0.0000252090
C 0.1374177302 1.2055629407
-0.0000531101
H -0.4093090904 2.1374462204
-0.0001029792
H 2.0593946796 2.1356466021
0.0001118293
H 3.2924886711 0.0000934029
0.0000305972
H 2.0595301725 -2.1355596379
0.0000023967
H -0.4091320475 -2.1375620896
-0.0000374218

case_studies/cuh_hydroamination/0.xyz

20
-51.79537150
H -0.0087947128 5.6461212714
0.0000126020
C -0.0072351041 4.5966125914
-0.0005088083
C -0.0050032456 3.3962797414

0.0004109512
C -0.0024770174 1.9814972114
0.0001178107
C -1.2072343783 1.2790407030
0.0167980493
C -1.1924971901 -0.1064904071
0.0198988088
C 0.0024144090 -0.8129237286
-0.0007579303
C 1.1949917099 -0.1020722001
-0.0208345790
C 1.2049277117 1.2833082899
-0.0167307284
H 2.1393438924 1.8237450187
-0.0321641274
C 2.5029710590 -0.8484495318
-0.0061221280
F 2.4124797579 -2.0644121315
-0.5578906786
F 2.9543562476 -1.0318113428
1.2487343523
F 3.4729475404 -0.1963495328
-0.6625595969
H 0.0045724476 -1.8919071686
-0.0013359107
C -2.5001129111 -0.8534534354
0.0059530174
F -2.3992836731 -2.0883273457
0.5111572570
F -2.9788798201 -0.9904842643
-1.2446749431

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 F          -3.4553131109        -0.2249824144
       0.7063951667
 H          -2.1437142577         1.8159110641
       0.0327514887

case_studies/cuh_hydroamination/3.xyz

  38
        -44.53477543
 H          -0.0002116757        -5.8361833046
      -0.0003430444
 C          -0.0001279641        -4.7870995701
      -0.0001097582
 C          -0.0000949970        -3.5865283456
       0.0001451633
 C          -0.0000087612        -2.1698046102
       0.0000274979
 C           1.2049961701        -1.4707819894
       0.0000231683
 C           1.2220097942        -0.0825707356
      -0.0000170849
 C           0.0000444286         0.5834933838
       0.0000134255
 C          -1.2219501847        -0.0825056598
      -0.0000962313
 C          -1.2049807291        -1.4707180617
      -0.0000627254
 H          -2.1317135336        -2.0254677907
      -0.0001291970
 SI         -2.8430247719         0.9082607712
      -0.0000024578
```

```
C          -4.3486456435       -0.2602302806
     -0.0061067888
H          -5.2756975684        0.3048524501
     -0.0075522677
H          -4.3549898198       -0.8982489622
     -0.8845386939
H          -4.3596389743       -0.9013123294
      0.8700434312
C          -2.8855446834        2.0119844925
     -1.5576986267
H          -2.8574698776        1.4170517656
     -2.4657540681
H          -3.7873936707        2.6160416488
     -1.5876505504
H          -2.0369572736        2.6886112344
     -1.5852956827
C          -2.8908457927        2.0029183911
      1.5639381272
H          -2.0420056530        2.6789125574
      1.5986806031
H          -3.7925045140        2.6072416226
      1.5940777450
H          -2.8664826978        1.4026071451
      2.4685580113
H           0.0000663978        1.6645040781
      0.0000833671
SI          2.8430793532        0.9081973789
     -0.0000191697
C           4.3488268115       -0.2601386708
     -0.0033060588
H           5.2758000186        0.3050717518
```

-0.0042378975
 H 4.3589287998 -0.9004241842
0.8734369220
 H 4.3562432326 -0.8989477431
-0.8811544232
 C 2.8895593083 2.0049575724
1.5624876550
 H 2.0403036746 2.6804897218
1.5960032899
 H 2.8651819973 1.4058164961
2.4678837349
 H 3.7908418808 2.6098597248
1.5922123262
 C 2.8866487932 2.0097831133
-1.5592011574
 H 2.8621307220 1.4133996530
-2.4664108142
 H 3.7871493350 2.6158952997
-1.5879450444
 H 2.0365396849 2.6843724488
-1.5898321996
 H 2.1317105538 -2.0255651255
0.0000308855

case_studies/cuh_hydroamination/ts2.xyz

195
symmetry c1
C -0.215070000 1.162880000
-3.358890000
C 0.085640000 -0.170800000

-3.774190000
H -0.758770000 -0.741390000
-4.158870000
H 0.567880000 1.912330000
-3.436930000
C 1.391540000 -0.456600000
-4.496670000
H 2.228350000 0.047900000
-4.002830000
H 1.614750000 -1.528500000
-4.537130000
H -1.234010000 1.525290000
-3.465010000
H 1.329820000 -0.073150000
-5.525240000
Cu 0.020990000 -0.008220000
-1.610150000
H 0.309690000 -1.299810000
-2.586880000
P 1.749770000 0.369300000
-0.170620000
C 1.187070000 1.286970000
1.345340000
C 3.122970000 1.401310000
-0.869670000
C 2.651870000 -1.096610000
0.499470000
C 0.205060000 0.722240000
2.224270000
C 1.674340000 2.579560000
1.586460000

```
C         4.469100000      1.066750000
-0.741620000
C         2.792530000      2.546990000
-1.610860000
C         2.612900000     -2.276870000
-0.237520000
C         3.390020000     -1.070370000
1.690890000
C        -0.168280000      1.527610000
3.292690000
C        -0.349260000     -0.672060000
2.211650000
C         1.252700000      3.374310000
2.665530000
H         2.424600000      2.989430000
0.921450000
C         5.495800000      1.784050000
-1.382100000
H         4.734040000      0.214090000
-0.130610000
C         3.756140000      3.305130000
-2.282020000
H         1.749740000      2.831180000
-1.667810000
C         3.354550000     -3.416590000
0.119670000
H         1.969590000     -2.300920000
-1.111610000
C         4.177890000     -2.154050000
2.093020000
H         3.346790000     -0.179850000
```

2.304940000
C 0.324240000 2.811300000
3.511640000
O -1.070150000 1.220300000
4.291610000
C -0.011570000 -1.480080000
3.290070000
C -1.282840000 -1.243660000
1.286530000
H 1.651110000 4.369310000
2.831450000
C 5.096760000 2.831720000
-2.239870000
C 4.223200000 -3.281390000
1.225330000
O -0.256040000 3.348090000
4.636880000
C -0.890830000 2.239160000
5.277160000
C -0.491090000 -2.774130000
3.474990000
O 0.841690000 -1.168340000
4.329810000
C -1.751700000 -2.549910000
1.488900000
P -1.787740000 -0.335750000
-0.253000000
H -1.863760000 2.548280000
5.661650000
H -0.241460000 1.859250000
6.080440000

C -1.364660000 -3.347710000 2.578630000
O 0.046790000 -3.311100000 4.621280000
C 0.630360000 -2.196540000 5.299000000
H -2.454730000 -2.968550000 0.778980000
C -3.119550000 -1.390070000 -0.997600000
C -2.729270000 1.131390000 0.357720000
H -1.746890000 -4.353650000 2.713800000
H -0.064740000 -1.832670000 6.070990000
H 1.587750000 -2.492190000 5.730100000
C -4.466050000 -1.318770000 -0.617470000
C -2.756440000 -2.307250000 -1.984170000
C -2.696500000 2.282030000 -0.426760000
C -3.481720000 1.145480000 1.539850000
C -5.461130000 -2.056420000 -1.265950000
H -4.738870000 -0.655160000 0.190790000
C -3.694340000 -3.117400000

-2.648620000
H -1.703370000 -2.382670000
-2.236870000
C -3.457440000 3.425040000
-0.126840000
H -2.040150000 2.281500000
-1.290480000
C -4.293670000 2.231940000
1.883860000
H -3.428430000 0.285830000
2.195590000
C -5.055550000 -2.877890000
-2.352910000
C -4.340340000 3.322350000
0.971280000
C 4.886730000 -2.142950000
3.472950000
C 4.400810000 -3.363360000
4.294700000
H 4.677820000 -4.303440000
3.813730000
H 4.846030000 -3.343870000
5.297750000
H 3.310260000 -3.346460000
4.404000000
C 6.429060000 -2.186460000
3.358840000
H 6.875840000 -2.035310000
4.349450000
H 6.784160000 -3.145760000
2.981850000

H 6.802110000 -1.389800000 2.703790000
C 4.531850000 -0.872960000 4.277640000
H 4.914540000 0.038170000 3.802940000
H 3.451650000 -0.760320000 4.414420000
H 4.993690000 -0.939600000 5.269490000
C 3.100200000 -4.707620000 -0.708170000
C 3.689800000 -4.548810000 -2.130020000
H 4.778550000 -4.424600000 -2.106390000
H 3.467850000 -5.437500000 -2.734030000
H 3.266910000 -3.678280000 -2.643180000
C 1.563910000 -4.904630000 -0.834850000
H 1.098670000 -4.994510000 0.153270000
H 1.071820000 -4.083870000 -1.362740000
H 1.357500000 -5.825440000 -1.393250000
C 3.634410000 -6.015810000 -0.080620000
H 4.721440000 -6.097730000

-0.101300000
H 3.307460000 -6.130070000
0.956940000
H 3.235720000 -6.861050000
-0.654830000
C -3.133470000 -4.214210000
-3.598430000
C -2.512810000 -3.564390000
-4.858000000
H -3.259130000 -3.012150000
-5.440110000
H -1.712720000 -2.865060000
-4.593490000
H -2.083430000 -4.335720000
-5.509470000
C -2.013460000 -4.980280000
-2.841980000
H -1.178280000 -4.338590000
-2.551060000
H -2.408330000 -5.453630000
-1.935580000
H -1.610000000 -5.770190000
-3.486530000
C -4.146750000 -5.297190000
-4.037140000
H -3.592800000 -6.104450000
-4.531850000
H -4.677050000 -5.727130000
-3.182690000
H -4.891140000 -4.936690000
-4.747740000

C -6.923350000 -2.023970000 -0.749550000
C -7.379320000 -3.464960000 -0.409770000
H -8.410550000 -3.452810000 -0.034710000
H -7.340040000 -4.113540000 -1.286880000
H -6.744070000 -3.898600000 0.371700000
C -7.900350000 -1.403700000 -1.776690000
H -7.546170000 -0.423920000 -2.118950000
H -8.040470000 -2.048210000 -2.644630000
H -8.883730000 -1.259160000 -1.312060000
C -7.047230000 -1.191730000 0.545770000
H -6.395540000 -1.569210000 1.341650000
H -6.813850000 -0.132860000 0.384970000
H -8.079350000 -1.249230000 0.909570000
C -3.206290000 4.686500000 -1.000590000
C -1.671460000 4.911120000 -1.092980000
H -1.240250000 5.061970000

-0.096780000
H -1.144930000 4.077290000
-1.563370000
H -1.467370000 5.806950000
-1.691310000
C -3.781990000 6.009640000
-0.444800000
H -4.869090000 6.071040000
-0.502250000
H -3.489320000 6.173300000
0.596160000
H -3.380470000 6.837200000
-1.042350000
C -3.754620000 4.457540000
-2.429350000
H -4.840690000 4.309790000
-2.427350000
H -3.536050000 5.325720000
-3.063560000
H -3.300820000 3.577100000
-2.897140000
C -5.024380000 2.268020000
3.252030000
C -4.537810000 3.509620000
4.041170000
H -4.798790000 4.435570000
3.524420000
H -4.999040000 3.528650000
5.037090000
H -3.449240000 3.486780000
4.168170000

C -4.697460000 1.019020000
4.099790000
H -5.077220000 0.098630000
3.640390000
H -3.622280000 0.900470000
4.265550000
H -5.181910000 1.116190000
5.078280000
C -6.564530000 2.324030000
3.115440000
H -7.025860000 2.196650000
4.102720000
H -6.904830000 3.279260000
2.715890000
H -6.936000000 1.518040000
2.471340000
C 6.955650000 1.371930000
-1.037470000
C 7.083910000 1.282980000
0.508970000
H 6.861040000 2.249750000
0.974540000
H 6.419110000 0.536320000
0.951630000
H 8.110800000 1.007390000
0.777000000
C 7.265370000 -0.020870000
-1.636450000
H 6.560660000 -0.778910000
-1.277070000
H 7.209790000 -0.010270000

-2.730880000
H 8.277410000 -0.339510000
-1.355980000
C 8.054190000 2.365600000
-1.481210000
H 9.001990000 2.058210000
-1.022390000
H 8.212250000 2.386690000
-2.559760000
H 7.836030000 3.385540000
-1.152700000
C 3.369480000 4.642400000
-2.966380000
C 1.890130000 5.002370000
-2.708500000
H 1.199860000 4.290110000
-3.173840000
H 1.657780000 5.057870000
-1.639500000
H 1.683560000 5.987420000
-3.141810000
C 3.561380000 4.607560000
-4.501240000
H 4.615040000 4.580380000
-4.780560000
H 3.054950000 3.742180000
-4.944980000
H 3.126980000 5.510880000
-4.947210000
C 4.228550000 5.783910000
-2.366310000

H 4.053720000 5.875470000
-1.287630000
H 5.294110000 5.612010000
-2.530610000
H 3.957120000 6.739980000
-2.831460000
O 5.138600000 -4.281300000
1.523320000
O 6.024470000 3.454000000
-3.063010000
O -6.052130000 -3.470140000
-3.115650000
O -5.269610000 4.323750000
1.216410000
C 6.321830000 2.720060000
-4.251520000
H 7.011640000 3.339070000
-4.831230000
H 6.800220000 1.759880000
-4.028050000
H 5.417190000 2.531230000
-4.840810000
C 6.308700000 -4.253060000
0.706470000
H 6.974410000 -5.028880000
1.094000000
H 6.078780000 -4.468130000
-0.342880000
H 6.810950000 -3.279870000
0.763280000
C -6.428050000 4.249210000

```
0.385730000
H       -7.097470000      5.047400000
0.717350000
H       -6.182540000      4.401440000
-0.671060000
H       -6.933200000      3.281880000
0.492230000
C       -6.282880000     -2.822840000
-4.367340000
H       -5.407690000     -2.880500000
-5.023380000
H       -7.118900000     -3.348590000
-4.836130000
H       -6.546730000     -1.767880000
-4.228370000

case_studies/cuh_hydroamination/1.xyz

  32
       -98.21273168
 H          -0.0011056489       -5.8849854205
      0.0068157265
 C          -0.0007005891       -4.8353441005
      0.0052367889
 C          -0.0002716193       -3.6350764305
      0.0034604716
 C          -0.0000673696       -2.2206286205
      0.0017845748
 C          -1.2089708497       -1.5263069008
      0.0388217665
 C          -1.1981296700       -0.1402438808
```

0.0419684697
C 0.0001217499 0.5609811795
-0.0009142088
C 1.1982792800 -0.1404962202
-0.0425727605
C 1.2089356203 -1.5265467502
-0.0366828937
H 2.1299141504 -2.0876133100
-0.0554477050
C 2.4992209599 0.6370143601
-0.0717127388
F 2.2756149596 1.9603904007
-0.3494946558
C 3.1794632100 0.5989980070
1.3231109510
F 3.3512797203 -0.6534191539
1.7509161581
F 4.3696500699 1.1894296773
1.3237773023
F 2.4144706300 1.2198359449
2.2180166025
C 3.4715160299 0.1295456228
-1.1689814201
F 4.3920900697 1.0381321536
-1.4608653381
F 2.8118443399 -0.1541715448
-2.2927342407
F 4.1092033501 -0.9837270179
-0.7979176627
H 0.0002000197 1.6391013895
-0.0019120664

```
 C          -2.4990468401          0.6373448588
       0.0697290416
 F          -2.2752813003          1.9615797483
       0.3431962446
 C          -3.1805824802          0.5950634219
      -1.3243492685
 F          -2.4165717904          1.2134455141
      -2.2217836171
 F          -4.3708914603          1.1852635617
      -1.3255473471
 F          -3.3526068500         -0.6585938072
      -1.7484106313
 C          -3.4702954899          0.1330912662
       1.1694346805
 F          -4.3903026701          1.0426913153
       1.4598974126
 F          -2.8094683398         -0.1478303263
       2.2932319198
 F          -4.1086427297         -0.9810207831
       0.8020138580
 H          -2.1300293096         -2.0872069611
       0.0587528553
```

case_studies/cuh_hydroamination/4.xyz

```
  24
        -33.66469221
 H          -5.3616726305          0.0001074295
      -0.3399227901
 C          -4.3165287005          0.0000751196
      -0.2496261402
```

```
C          -3.1206415105          0.0000882496
     -0.1443893302
C          -1.7099197505          0.0000266497
     -0.0231043503
C          -1.0118167806          1.2027331297
      0.0419923999
C           0.3684587594          1.2163381698
      0.1559997398
C           1.0554476195         -0.0000486702
      0.2018860395
C           0.3683946996         -1.2163763302
      0.1560369892
C          -1.0119222904         -1.2027119403
      0.0423024393
H          -1.5558152603         -2.1357381103
      0.0062179492
C           1.1100202197         -2.5175176502
      0.2315262389
H           1.2608040197         -2.9276940299
     -0.7680924312
H           0.5435907998         -3.2443183503
      0.8095372788
H           2.0817887797         -2.3709701902
      0.6964233989
O           2.4384327095         -0.0000905101
      0.3389513394
C           3.1311374894          0.0001081202
     -0.8894786307
H           2.8959992695         -0.8899429896
     -1.4834603409
H           2.8962225293          0.8904657204
```

```
      -1.4830752205
 H           4.1915506595        -0.0000828797
      -0.6417877407
 C           1.1101872194         2.5173944198
       0.2317612500
 H           1.2625285593         2.9269972701
      -0.7678542699
 H           2.0812772194         2.3709058898
       0.6981094699
 H           0.5430747293         3.2446207297
       0.8085565402
 H          -1.5556548306         2.1357841397
       0.0055785601

case_studies/pd_diarylation/2.xyz

  18
        -27.32987487
 H           3.3565357472        -2.5600592292
       0.0002282098
 C           2.4312936141        -2.0660734850
       0.0001757998
 C           1.3772833104        -1.4916440917
       0.0000565098
 C           0.1233267063        -0.8363904596
      -0.0000879203
 C           0.0677773674         0.5712950000
      -0.0001046107
 C          -1.1717631866         1.1968764322
       0.0001321693
 C          -2.3358423718         0.4440294248
```

0.0000761697
C -2.2831180731 -0.9379037649
-0.0000510999
C -1.0551112790 -1.5740791671
-0.0000361399
H -0.9935599922 -2.6523659167
0.0000091104
H -3.1934740294 -1.5178071306
-0.0000901597
H -3.2898971250 0.9502464688
0.0002952696
H -1.2439501234 2.2733690617
0.0003113490
O 1.2669353133 1.2141284276
-0.0003748610
C 1.2795020544 2.6191759777
0.0001906485
H 0.7953894517 3.0278408943
-0.8931364115
H 0.7964027020 3.0270596549
0.8944359385
H 2.3307938826 2.9027183743
-0.0002918517

case_studies/pd_diarylation/5.xyz

17
-23.26874095
H 4.4028664502 1.0284242383
-0.0004827355
C 3.4008938900 0.7176604990

-0.0000463241
C 2.2545447698 0.3612609297
-0.0000236526
C 0.9018572695 -0.0581315993
0.0001491493
C -0.1213379599 0.8894115014
-0.0000289809
C -1.4493544101 0.4965094823
-0.0003333091
C -1.7470847411 -0.8631271575
-0.0002473471
C -0.7370867417 -1.8088636982
0.0000713031
C 0.5880344986 -1.4157625691
0.0001777713
H 1.3821890081 -2.1477805497
0.0002292415
H -0.9850703124 -2.8605160181
0.0001172647
H -2.7806911913 -1.1789528568
-0.0004549557
C -2.5554804094 1.5079863930
0.0001636807
H -3.1941642004 1.3715385424
-0.8718131285
H -2.1593927688 2.5202275027
-0.0139947109
H -3.1760211987 1.3896790246
0.8878837515
H 0.1349306709 1.9396663012
-0.0000820025

case_studies/pd_diarylation/16.xyz

```
 14
       -27.25714825
H          -0.0002676155          5.7320838391
     -0.0000486990
C          -0.0001110661          4.6828443891
     -0.0000056287
C          -0.0000718768          3.4826013791
      0.0000120816
C          -0.0000059976          2.0673751991
      0.0000013119
C           1.2089169920          1.3716177284
     -0.0000161283
C           1.1891643912         -0.0105168916
     -0.0000003680
C           0.0000186707         -0.7220838009
      0.0000201925
C          -1.1891384088         -0.0105545002
      0.0000136027
C          -1.2089014280          1.3715833598
      0.0000103924
H          -2.1433535677          1.9107739603
      0.0000080325
BR         -2.8355762694         -0.9683330493
     -0.0000040866
H           0.0000327101         -1.8005895809
      0.0000562828
BR          2.8355986506         -0.9682822926
     -0.0000013982
```

```
 H           2.1433481223         1.9108306878
      -0.0000033187

case_studies/pd_diarylation/14.xyz

  20
        -51.79537145
 H           0.0092567661         5.6463450585
       0.0007200432
 C           0.0074697696         4.5968341097
       0.0000412505
 C           0.0057685010         3.3964926245
       0.0000879795
 C           0.0029687889         1.9817095056
      -0.0001503293
 C           1.2074520769         1.2788446918
       0.0166080725
 C           1.1922272229        -0.1067114371
       0.0198095523
 C          -0.0029128895        -0.8126789440
      -0.0007496026
 C          -1.1952805432        -0.1013846420
      -0.0210036186
 C          -1.2047266617         1.2839533031
      -0.0170593325
 H          -2.1388934186         1.8248047173
      -0.0326520675
 C          -2.5030413023        -0.8481564793
      -0.0061131705
 F          -2.4143674719        -2.0598707274
      -0.5675709328
```

```
 F          -2.9485924260       -1.0414464604
      1.2493300049
 F          -3.4762652786       -0.1916659912
     -0.6531655553
 H          -0.0055415302       -1.8916631370
     -0.0012263623
 C           2.4998020118       -0.8538035641
      0.0059384685
 F           3.4535973748       -0.2276194909
      0.7103636596
 F           2.9810209253       -0.9866242671
     -1.2441510797
 F           2.3979810335       -2.0902967545
      0.5068649008
 H           2.1441569733        1.8153322831
      0.0325342937

case_studies/pd_diarylation/6.xyz

  20
        -29.69283196
 H          -5.3448123089       -0.9022035228
      0.0000449809
 C          -4.3292746190       -0.6391269726
     -0.0000544491
 C          -3.1658482891       -0.3426901823
     -0.0000488991
 C          -1.7969938792        0.0180609281
      0.0000286410
 C          -1.4399974095        1.3864042181
      0.0000466701
```

```
C          -0.1269347096          1.7537964885
      0.0000348001
C           0.8999775307          0.7844606887
      0.0000010010
C           2.2645476906          1.1372469090
     -0.0000437490
C           3.2351926008          0.1746378493
     -0.0000464381
C           2.8852540811         -1.1849860808
     -0.0000081973
C           1.5714062312         -1.5600451511
      0.0000304327
C           0.5451631110         -0.5910810614
      0.0000239119
C          -0.8160863189         -0.9477461317
      0.0000269418
H          -1.0882622687         -1.9939797618
      0.0000174025
H           1.2968043915         -2.6054893012
      0.0000457634
H           3.6656057313         -1.9321038106
      0.0000977934
H           4.2791098207          0.4525933795
     -0.0000451281
H           2.5292232603          2.1853477191
     -0.0001011496
H           0.1479706202          2.7993001685
     -0.0000012605
H          -2.2252589597          2.1284368379
      0.0000528294
```

case_studies/pd_diarylation/12.xyz

```
  26
        -41.78396972
 H          -5.1959488955          1.6765876813
       0.1396675734
 C          -4.2027782344          1.3408047448
       0.1054866128
 C          -3.0661523131          0.9555499687
       0.0662958020
 C          -1.7264207215          0.5027468134
       0.0209257712
 C          -1.4546414968         -0.8631548056
      -0.0009499092
 C          -0.1420256053         -1.2979091510
      -0.0339883001
 C           0.9232512515         -0.3722913473
      -0.0543984705
 C           0.6355466167          1.0009538417
      -0.0563198700
 C          -0.6867248747          1.4241740971
      -0.0062459092
 H          -0.9312513584          2.4735881762
      -0.0001704388
 O           1.6943551836          1.8740941154
      -0.1203790605
 C           1.4326673388          3.2538812045
      -0.0758596400
 H           2.4094096671          3.7345935079
      -0.1146236205
 H           0.8365107272          3.5810276426
```

```
      -0.9339055196
 H          0.9259663484          3.5411840125
       0.8512639603
 O          2.1589030435         -0.9479765930
      -0.1103876113
 C          3.2942930713         -0.2478877691
       0.3429444482
 H          3.1235929002          0.2070286601
       1.3220032384
 H          3.6059192382          0.5254923221
      -0.3624906418
 H          4.0779952140         -1.0012097464
       0.4263853576
 O          0.2407500893         -2.6056045897
      -0.0437296906
 C         -0.7594734173         -3.5920001332
      -0.0439832702
 H         -1.3786729269         -3.5420426655
       0.8583986202
 H         -1.4017111680         -3.5171372052
      -0.9279944298
 H         -0.2311161840         -4.5439311613
      -0.0639944907
 H         -2.2777398943         -1.5584153985
       0.0178693011
```

case_studies/pd_diarylation/10.xyz

```
  17
       -35.94904685
 H         -1.3428379999          3.8412739431
```

```
      0.0000482247
C          -0.7276226220          2.9916666316
      0.0000927237
C          -0.0309788744          2.0142585899
     -0.0000285274
C           0.7939208727          0.8653710078
      0.0000482312
C           0.2369211995         -0.4203527008
      0.0000974801
C           1.0537863367         -1.5400884029
      0.0001077488
C           2.4301077871         -1.3897535963
      0.0000606386
C           2.9903694502         -0.1219436577
     -0.0000674303
C           2.1821296930          0.9984248343
     -0.0000521690
H           2.6109199955          1.9890134832
     -0.0001885382
H           4.0638938605         -0.0071832904
     -0.0000861205
H           3.0626866649         -2.2636142579
      0.0001191175
H           0.6117921742         -2.5245553818
      0.0001268580
C          -1.2585816109         -0.5657457971
     -0.0000062296
F          -1.8346378998          0.0010611654
     -1.0765293089
F          -1.8348719592          0.0012828533
      1.0762859311
```

```
 F          -1.6573915141       -1.8475680161
       0.0000827293

case_studies/pd_diarylation/7.xyz

  18
        -27.33163774
 H           4.2557687877        2.0397357630
      -0.0006591289
 C           3.3860126765        1.4531250771
      -0.0001631846
 C           2.3932905157        0.7781203752
       0.0000248294
 C           1.2194306803       -0.0146209760
       0.0001568059
 C          -0.0279047411        0.6117139187
       0.0001935418
 C          -1.1836888244       -0.1553019019
       0.0000436429
 C          -1.0841212644       -1.5489891308
      -0.0001734125
 C           0.1531743158       -2.1599043931
      -0.0000799201
 C           1.3118834199       -1.4031757979
       0.0001151286
 H           2.2826357831       -1.8751162583
       0.0002040960
 H           0.2155792693       -3.2380400752
      -0.0001909421
 H          -1.9949374802       -2.1263225043
      -0.0004403420
```

```
 O          -2.4506154213          0.3465390205
       0.0000608511
 C          -2.6208387319          1.7423549770
      -0.0001011540
 H          -2.1854733064          2.2014195550
       0.8936649177
 H          -3.6970760715          1.9080249480
      -0.0007430547
 H          -2.1843951737          2.2013882076
      -0.8933593561
 H          -0.0629717393          1.6901617514
       0.0003638838

case_studies/pd_diarylation/0.xyz

  14
        -28.19977064
 H           0.0004077611          3.9452194477
       0.0000216553
 C           0.0003171108          2.8962499277
       0.0000416460
 C           0.0001181505          1.6959943677
       0.0000561669
 C          -0.0000050298          0.2829717077
       0.0000359180
 C          -1.1993371200         -0.4373021120
       0.0000377884
 C          -1.2030548404         -1.8210809020
       0.0000222495
 C          -0.0001321206         -2.5070987423
       0.0000151901
```

```
 C           1.2028833996       -1.8211751226
      0.0000303797
 C           1.1993145100       -0.4374342626
     -0.0000050513
 CL          2.6936157302        0.4256466070
     -0.0000371319
 H           2.1414301895       -2.3517186029
      0.0000142102
 H          -0.0001795408       -3.5858471423
     -0.0000374291
 H          -2.1416965605       -2.3514543118
     -0.0000269002
 CL         -2.6936498998        0.4258541384
     -0.0000414323

case_studies/pd_diarylation/3.xyz

  23
        -29.61069865
 H           4.4676072807        0.0011164829
      0.0069721974
 C           3.4185747707        0.0005853920
      0.0050365777
 C           2.2176570707        0.0006522809
      0.0026728281
 C           0.8018912307        0.0001645597
      0.0004326985
 C           0.1082008418       -1.2162120509
     -0.0014081119
 C          -1.2759956982       -1.1957713120
     -0.0056357915
```

```
C          -1.9835827393       -0.0008723126
     -0.0083589807
C          -1.2766954003        1.1946963380
     -0.0055963503
C           0.1073176597        1.2161778191
     -0.0013831207
C           0.8645059486        2.5087292298
     -0.0007288503
H           1.5062790183        2.5722929408
     -0.8791116104
H           1.5074588788        2.5706910199
      0.8768750396
H           0.1843929579        3.3569965292
      0.0004238203
H          -1.8192104211        2.1301498575
     -0.0078968297
C          -3.4820840293       -0.0001501039
      0.0104407698
H          -3.8764323302        0.8721650660
     -0.5061492597
H          -3.8413658090        0.0278341953
      1.0401064199
H          -3.8772346386       -0.8980612040
     -0.4592773206
H          -1.8175304174       -2.1317880425
     -0.0080503418
C           0.8662425329       -2.5082652502
     -0.0006989628
H           1.5088093427       -2.5710194892
     -0.8785460230
H           0.1867613036       -3.3570270108
```

```
      -0.0004547530
 H          1.5085116532       -2.5701874901
       0.8774015770

case_studies/pd_diarylation/8.xyz

  14
        -28.55576548
 H          4.8001171695        0.0000283979
      -0.0000876003
 C          3.7508984895       -0.0000339862
      -0.0000027004
 C          2.5505952195       -0.0000111908
       0.0000290395
 C          1.1350229695       -0.0000229562
      -0.0000015607
 C          0.4396761948        1.2088853511
       0.0000139301
 C         -0.9408618651        1.1820987157
       0.0000112299
 C         -1.6613262405        0.0000193430
       0.0000212891
 C         -0.9408861459       -1.1820796943
      -0.0000105116
 C          0.4396479242       -1.2089164389
      -0.0000392815
 H          0.9657799278       -2.1500504669
      -0.0000549821
 F         -1.6146562914       -2.3464281969
       0.0000109575
 H         -2.7385863205        0.0000118888
```

```
      -0.0000212210
 F          -1.6145844496          2.3464676131
      -0.0000176494
 H           0.9658515512          2.1499924231
       0.0000345107

case_studies/pd_diarylation/15.xyz

  14
        -28.20076541
 H           0.0034241422         -5.1912476004
      -0.0000830917
 C           0.0027393917         -4.1419672804
      -0.0000438116
 C           0.0018425326         -2.9416311203
       0.0000191285
 C           0.0009202755         -1.5258620603
       0.0000290086
 C           1.2100620718         -0.8314262413
       0.0000555184
 C           1.1924315344          0.5517020688
       0.0000272185
 C          -0.0007931092          1.2588796397
      -0.0000192711
 C          -1.1931572756          0.5502149505
      -0.0000047908
 C          -1.2090958182         -0.8329050693
      -0.0000168110
 H          -2.1426466731         -1.3727844508
      -0.0000321808
 CL         -2.6853181477          1.4183505241
```

```
       0.0000017597
 H          -0.0014425794          2.3365181097
       0.0000029790
 CL          2.6835373423          1.4216010053
      -0.0000172618
 H           2.1443214369         -1.3700823198
       0.0001071481

case_studies/pd_diarylation/1.xyz

  14
        -32.77705497
 H           4.5341649000         -0.0000854703
       0.0002316767
 C           3.4853398900         -0.0000210280
       0.0000251374
 C           2.2853634200          0.0000432245
       0.0000536281
 C           0.8723978600          0.0000306075
      -0.0000222709
 C           0.1399057825          1.1906304391
      -0.0000208796
 C          -1.2412758474          1.2117295321
       0.0000118113
 C          -1.9105797500         -0.0000313265
       0.0000057408
 C          -1.2412249826         -1.2117638879
      -0.0000221705
 C           0.1399531075         -1.1906038809
      -0.0000224114
 F           0.7999326650         -2.3569299223
```

```
      -0.0000214227
 H         -1.7780997746        -2.1459108568
      -0.0000244409
 F         -3.2510584100        -0.0000598837
       0.0000389617
 H         -1.7782000754         2.1458483532
       0.0000367223
 F          0.7998302350         2.3569890077
      -0.0000359091

case_studies/pd_diarylation/13.xyz

  16
        -30.55747121
 H         -4.6910420907        -1.8798830909
      -0.0007003887
 C         -3.7963621308        -1.3317809108
      -0.0004011790
 C         -2.7704672008        -0.7088008908
       0.0001186406
 C         -1.5636634808         0.0315976693
       0.0001616601
 C         -1.5940034509         1.4287070493
       0.0000313387
 C         -0.4168475909         2.1563624293
       0.0000237782
 C          0.8049840891         1.5075342394
       0.0000149691
 C          0.8296639092         0.1173761894
       0.0001064604
 C         -0.3383903008        -0.6295086007
```

0.0002865509
H -0.2878381107 -1.7078011407
0.0004667920
N 2.1013701392 -0.5660492906
0.0000016613
O 3.1047455092 0.1144098795
-0.0003769092
O 2.0890088493 -1.7782014006
0.0001465325
H 1.7361549391 2.0524147394
-0.0000926213
H -0.4514749209 3.2348713093
-0.0000813328
H -2.5483683109 1.9337112192
-0.0000367119

case_studies/pd_diarylation/4.xyz

20
-26.43951496
H 4.7312656271 -0.0069528320
-0.0013309013
C 3.6822150789 -0.0049882014
-0.0008574833
C 2.4817304014 -0.0043080894
-0.0002153755
C 1.0654459937 -0.0019401836
0.0001579200
C 0.3699503922 1.2044848857
0.0077877355
C -1.0164181155 1.2131511325

```
      0.0093862211
C          -1.6958457472          0.0021344608
      0.0025286810
C          -1.0188136147         -1.2120770856
     -0.0054935990
C           0.3661164584         -1.2075795885
     -0.0064169515
H           0.9157488206         -2.1380460156
     -0.0113740441
C          -1.7864046359         -2.4998774256
      0.0021209003
H          -2.5719626177         -2.4823727769
     -0.7514909978
H          -1.1315085917         -3.3453763576
     -0.1930811221
H          -2.2594718823         -2.6485691150
      0.9730126976
H          -2.7772718140          0.0019585748
      0.0040140000
C          -1.7710957862          2.5084565860
     -0.0066144449
H          -2.7102899689          2.4169308897
      0.5345759976
H          -2.0013750721          2.7916722010
     -1.0344811623
H          -1.1822561645          3.3068537716
      0.4389463779
H           0.9208345457          2.1342122935
      0.0128040912
```

case_studies/pd_diarylation/11.xyz

```
 22
       -34.56514110
H          3.9043400047       -3.3107300001
      0.0000615176
C          3.0899540313       -2.6493963289
      0.0000438102
C          2.1516292006       -1.9008016825
      0.0000211367
C          1.0558711559       -1.0026600670
     -0.0000130156
C          1.3024783390        0.3730470652
      0.0000413663
C          0.2309528728        1.2496676195
     -0.0000230468
C         -1.0783833735        0.7612102899
     -0.0000730552
C         -1.3161392354       -0.6039428119
     -0.0000636270
C         -0.2403676464       -1.4924216494
     -0.0000711564
H         -0.4332895480       -2.5528340868
     -0.0000950120
O         -2.5521154073       -1.1736398091
     -0.0000488683
C         -3.6792091778       -0.3320896721
      0.0001462321
H         -4.5424128847       -0.9959020127
      0.0003168075
H         -3.7085448245        0.3001209599
      0.8933882789
```

```
 H          -3.7088877754          0.3001018563
      -0.8930962723
 H          -1.8747524987          1.4865016316
      -0.0001235078
 O           0.3357073628          2.6092447780
      -0.0000487479
 C           1.6204601806          3.1814694082
       0.0000531740
 H           2.1867136443          2.8987850532
       0.8934338310
 H           2.1869051102          2.8986734745
      -0.8931696905
 H           1.4631999119          4.2590024427
      -0.0000290755
 H           2.3238644805          0.7176408415
       0.0001260022

case_studies/pd_diarylation/9.xyz

  20
         -29.69310222
 H          -3.8783403647          2.5708338323
       0.0001854769
 C          -3.1470309233          1.8186055837
       0.0000769869
 C          -2.3055706516          0.9614491953
       0.0000240670
 C          -1.3344212996         -0.0675498928
      -0.0000362330
 C          -1.7369828771         -1.3859297536
      -0.0000778340
```

```
C          -0.7928985351       -2.4183788218
     -0.0000364640
C           0.5453629544       -2.1345769792
      0.0000543070
C           0.9986084518       -0.7985877383
      0.0000388280
C           2.3727365112       -0.4787014957
      0.0000614590
C           2.7889035487        0.8228242251
     -0.0000006600
C           1.8497220067        1.8653602433
     -0.0000547600
C           0.5105049472        1.5895875407
     -0.0000426010
C           0.0511433498        0.2573945498
     -0.0000127520
H          -0.2188084543        2.3868250393
     -0.0000722410
H           2.1941459747        2.8892104740
     -0.0001116193
H           3.8432207382        1.0585696272
      0.0000034307
H           3.0911409427       -1.2864029443
      0.0001156290
H           1.2765577159       -2.9303831178
      0.0001157370
H          -1.1337484831       -3.4435704624
     -0.0000494347
H          -2.7917200566       -1.6204235956
     -0.0001195747
```

case_studies/2,1,3-benzoselenodiazole.xyz

13
Coordinates from ORCA-job
/scratch/83610694.tmpdir/opt1_pbe_tzvp
  Se  5.73336180043050      4.45186661471386
    -0.00062892490819
  N   4.87248509662184      5.97627569402367
    0.41208506307863
  N   4.44698848548226      3.35320496413990
    0.61033647671116
  C   2.72157952449145      6.50719540991555
    1.43809888576155
  C   1.56801794110931      6.00385287941530
    1.98668023601455
  C   1.33957561486293      4.59650917024067
    2.09269404000838
  C   2.26302565344281      3.68151365399251
    1.65110970612690
  C   3.47877879099971      4.15506437866459
    1.07300762228373
  C   3.71257370822620      5.59627318578889
    0.96411430981213
  H   2.09571542883677      2.60697445152264
    1.72881241049703
  H   0.40553722777671      4.24806069681822
    2.53691231184786
  H   0.80183770574071      6.68930474340865
    2.35314545770449
  H   2.90243876397880      7.57905204835556
    1.35397888906178

```
case_studies/2,1,3-benzothiadiazole.xyz

13
Coordinates from ORCA-job
/scratch/83610661.tmpdir/opt1_pbe_tzvp
  S   -2.1923621961406
-0.0083948290251 2     -0.0051299175826 7
  N   -1.1723711715274
8 1.2579993213061 1      0.0029570680502 6
  N   -1.1627020885222
2 -1.2669445191585 2     -0.0127313925667 4
  C   0.07152959093745      0.72516350775175
    -0.00014786704439
  C   0.07707002749118     -0.72463126198437
    -0.00919776121508
  C   1.30573356226469     -1.43354635204427
    -0.01340124876381
  C   2.47386253036571     -0.70332074514135
    -0.00866666314621
  C   2.46834370874596      0.72250952075065
     0.00020532476937
  C   1.29462133166205      1.44366896933368
     0.00451578596964
  H   1.30443090520299     -2.52362847805092
    -0.02017533102597
  H   3.43296704221563     -1.22397744573040
    -0.01174788601182
  H   3.42353547085587      1.25027359954276
     0.00364133909409
  H   1.28466904092222      2.53372548944999
```

0.01130807747333

case_studies/au_nhc.xyz

23
symmetry c1
Cl 3.648910628 0.079101578 0.025091797
Au 1.313139146 -0.019287551 -0.005245302
C -0.668616752 -0.048238052 0.003640023
N -1.477269470 -1.089697950 -0.005876954
N -1.452910738 1.080574742 -0.008090534
C -2.816011636 -0.682734416 0.003093482
C -1.059764268 -2.489290645 0.004117584
C -2.799274260 0.697829867 0.025704626
C -4.035708740 -1.394124365 -0.011296507
C -3.960808117 1.454936025 0.023997203
C -0.974566526 2.431252530 -0.027674745
H -1.721284243 3.034910222 -0.033252916
H -0.444245050 2.571048113

```
-0.815461772
H       -0.437716606      2.591603005
0.751916584
C       -5.139591037      0.775969116
0.017808918
H       -3.933843274      2.383605212
0.024897876
C       -5.176736431     -0.652137530
-0.004768348
H       -5.938631330      1.252258346
0.029691654
H       -5.999364427     -1.084356923
-0.016069232
H       -4.058603511     -2.323523631
-0.024405363
H       -1.835727551     -3.054230646
-0.011321102
H       -0.551224823     -2.666002221
0.798469706
H       -0.518476412     -2.666502371
-0.768128871


case_studies/ethene_dimer.xyz

12
symmetry c1
C        0.000000000     -0.666365290
0.000000000
C        0.000000000      0.666365290
0.000000000
```

```
H         0.000000000     -1.240594776
0.928733148
H         0.000000000     -1.240594768
-0.928733151
H         0.000000000      1.240594768
0.928733151
H         0.000000000      1.240594776
-0.928733148
C        -0.666365290      0.000000000
3.800000000
C         0.666365290      0.000000000
3.800000000
H        -1.240594776      0.000000000
4.728733148
H        -1.240594768      0.000000000
2.871266849
H         1.240594768      0.000000000
4.728733151
H         1.240594776      0.000000000
2.871266852
```

case_studies/perfluoropropane.xyz

```
11
Coordinates from ORCA-job
/scratch/83611028.tmpdir/opt1_pbe_tzvp
  C   0.0228782095946     -0.0475508463172
5
    -2.56606848149340
  F   -0.638608388602 10
0.99602327842481     -2.03431749279903
```

```
  F   -0.62827448452437
-1.18058696110618     -2.24669891721228
  F   1.25955163722328      -0.09596590650220
    -2.03886855501404
  C   0.08858592839738       0.07318629819669
    -4.12626108074448
  F   0.72904856942613      -1.02437543125113
    -4.60315877578121
  F   -1.18417199722122
0.08627759634569     -4.59753559584471
  C   0.82215057800199       1.33918227531045
    -4.68498222140840
  F   0.21369079439735       2.46493289831609
    -4.27025917236746
  F   2.10580982454966       1.36256341231480
    -4.28366636401756
  F   0.78984642475244       1.29999694626823
    -6.02930264831742

case_studies/2,1,3-benzotellurodiazole.xyz

13
Coordinates from ORCA-job
/scratch/83610660.tmpdir/opt1_pbe_tzvp
  C   -2.43559784069397
1.42873381136349      0.00047910155702
  C   -1.17814523508466
0.73981320008690      0.00138227741067
  C   -1.17503603665357
-0.73837962753181       0.00120043958329
  N   -0.01872905846433
```

```
1.3995591052477 5      0.0023693654155 1
  C   -3.6028346024727 9
0.7111012598722 3     -0.0005407845027 3
  H   -2.4281550941995 8
2.5191498901705 7      0.0006071573229 6
  C   -3.5998073851557 5
-0.7200888937347 1     -0.0007130553403 6
  H   -4.5596759585264 5
1.2363746483384 4     -0.0012278298634 9
  C   -2.4294938858577
-1.4327055616547 0      0.0001332115151 4
  H   -4.5544013467568 3
-1.2494214635882 8     -0.0015590936102 9
  H   -2.4173282817889 0
-2.5230789710287 6      0.0000225289477 1
  N   -0.0127847972391 1
-1.3931308613027 3      0.0020357436504 3
  Te  1.4036879496217 2      0.0061581217616 1
     0.0032202629141 3

case_studies/corannulene.xyz

30
Coordinates from ORCA-job
/scratch/85243210.tmpdir/opt1_pbe_tzvp
  C   0.9295959514589 3      0.9035273096917 7
    -0.8511117437283 8
  C   -0.4512899232015 2
1.2227767757344 4     -0.8255041780597 6
  C   -1.1819323648477 8
0.0080553613537 4     -0.8315632868605 6
```

```
  C   -0.25261011544397
-1.06192600058624     -0.86097473480956
  C   1.05238499926284     -0.50854431522922
    -0.87295736069601
  C   2.15812053701117     -1.17627509289550
    -0.36091455274601
  C   3.26430983989744     -0.31675291807276
    -0.00592133896934
  C   3.14378762771754      1.06967373052346
     0.01552032663817
  C   1.90495352754654      1.73593681807382
    -0.31584084964361
  C   1.42851146896866      3.04467274906714
     0.06967029288613
  C   0.07269528501688      3.35810921711707
     0.09481191460386
  C   -0.94290306779111
2.39436226981850     -0.26305059513325
  C   -2.33599639180489
2.33675701978223      0.11697210201305
  C   -3.05334901040827
1.14405612760320      0.11106404232344
  C   -2.44974856973089
-0.11078135901640     -0.27558249559358
  C   -2.82676214290516
-1.46225007482151      0.07059552334365
  C   -1.91434440600950
-2.51288317604368      0.04168353126457
  C   -0.53324583375267
-2.31759429682759     -0.33627853725941
  C   0.63438052034408     -3.10221224382273
```

```
    -0.00551992426478
  C   1.91568199984792     -2.55883051911721
    -0.01718519348232
  H   4.19688559956741     -0.76174693345344
     0.35008595621305
  H   3.98656263601534      1.65773623394901
     0.38750439806890
  H   2.13895087952221      3.78509571060262
     0.44585673974676
  H   -0.22717050348917
4.33207355569347      0.48970407050174
  H   -2.82156642246099
3.23199866966452      0.51349088847602
  H   -4.07352053276158
1.15055882943493      0.50307799162623
  H   -3.82939143384747
-1.65670291942405      0.45967958039285
  H   -2.23710310568101
-3.49024960815411      0.40916661553536
  H   0.50817872079750     -4.12496355051683
     0.35850171267543
  H   2.74422423116145     -3.17673737012869
     0.33801910493721

case_studies/tris(3,5-tert-butylphenyl)metha
ne_dimer.xyz

214
sr220_xl_can
C      11.311007    6.044559   16.012442
C      13.845329    6.014571   15.944521
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| C | 11.207935 | 1.727216 | 16.426918 |
| C | 10.062614 | 4.010508 | 16.255924 |
| C | 10.024285 | 1.110566 | 15.666681 |
| C | 12.457321 | 3.930870 | 16.125047 |
| C | 8.811043 | 6.265997 | 16.114919 |
| C | 7.530477 | 5.450748 | 16.305375 |
| C | 11.248647 | 3.251264 | 16.243809 |
| C | 12.495650 | 5.326425 | 16.014626 |
| C | 11.054815 | 1.432495 | 17.929915 |
| C | 8.728426 | 6.978769 | 14.754714 |
| C | 10.073537 | 5.400503 | 16.139942 |
| C | 8.887107 | 7.317579 | 17.239188 |
| C | 12.491679 | 1.050787 | 15.920292 |
| H | 11.354103 | 7.123349 | 15.905397 |
| H | 13.397091 | 3.386907 | 16.125643 |
| H | 14.473697 | 5.386203 | 15.316153 |
| H | 9.112318 | 3.499314 | 16.360586 |
| H | 6.665578 | 6.118438 | 16.274989 |
| H | 7.401189 | 4.713747 | 15.521505 |
| H | 7.521739 | 4.940547 | 17.267984 |
| H | 10.045535 | 0.022442 | 15.756845 |
| H | 7.989042 | 7.933633 | 17.242365 |
| H | 12.387613 | -0.031180 | 16.018995 |
| H | 7.836915 | 7.609122 | 14.709831 |
| H | 8.668846 | 6.245740 | 13.945622 |
| H | 9.598687 | 7.608526 | 14.576769 |
| H | 10.139075 | 1.862859 | 18.315396 |
| H | 12.686107 | 1.272622 | 14.872086 |
| H | 9.738501 | 7.981495 | 17.112879 |
| H | 8.970717 | 6.836771 | 18.209741 |
| H | 13.373458 | 1.343721 | 16.487490 |

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| H | 9.061874 | 1.442822 | 16.053949 |
| H | 11.886150 | 1.846375 | 18.493340 |
| H | 11.024230 | 0.351917 | 18.110839 |
| H | 10.066983 | 1.360800 | 14.607751 |
| C | 13.777408 | 8.548893 | 15.974509 |
| C | 13.362932 | 8.651965 | 11.657166 |
| C | 13.533926 | 9.797286 | 13.940458 |
| C | 14.123169 | 9.835615 | 11.040516 |
| C | 13.664803 | 7.402579 | 13.860820 |
| C | 13.674931 | 11.048857 | 16.195947 |
| C | 13.484475 | 12.329423 | 15.380698 |
| C | 13.546041 | 8.611253 | 13.181214 |
| C | 13.775224 | 7.364250 | 15.256375 |
| C | 11.859935 | 8.805085 | 11.362445 |
| C | 15.035136 | 11.131474 | 16.908719 |
| C | 13.649908 | 9.786363 | 15.330453 |
| C | 12.550662 | 10.972793 | 17.247529 |
| C | 13.869558 | 7.368221 | 10.980737 |
| H | 13.884453 | 8.505797 | 17.053299 |
| H | 13.664207 | 6.462809 | 13.316857 |
| H | 13.429264 | 10.747582 | 13.429264 |
| H | 13.514861 | 13.194322 | 16.048388 |
| H | 14.268345 | 12.458711 | 14.643697 |
| H | 12.521866 | 12.338161 | 14.870497 |
| H | 14.033005 | 9.814365 | 9.952392 |
| H | 12.547485 | 11.870858 | 17.863583 |
| H | 13.770855 | 7.472287 | 9.898770 |
| H | 15.080019 | 12.022985 | 17.539072 |
| H | 15.844228 | 11.191054 | 16.175690 |
| H | 15.213081 | 10.261213 | 17.538476 |
| H | 11.474454 | 9.720825 | 11.792809 |

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| H | 14.917764 | 7.173793 | 11.202572 |
| H | 12.676971 | 10.121399 | 17.911445 |
| H | 11.580109 | 10.889183 | 16.766721 |
| H | 13.302360 | 6.486442 | 11.273671 |
| H | 13.735901 | 10.798026 | 11.372772 |
| H | 11.296510 | 7.973750 | 11.776325 |
| H | 11.679011 | 8.835670 | 10.281867 |
| H | 15.182099 | 9.792917 | 11.290750 |
| C | 13.815341 | 6.082492 | 18.478843 |
| C | 18.132684 | 6.496968 | 18.581915 |
| C | 15.849392 | 6.325974 | 19.727236 |
| C | 18.749334 | 5.736731 | 19.765565 |
| C | 15.929030 | 6.195097 | 17.332529 |
| C | 13.593903 | 6.184969 | 20.978807 |
| C | 14.409152 | 6.375425 | 22.259373 |
| C | 16.608636 | 6.313859 | 18.541203 |
| C | 14.533475 | 6.084676 | 17.294200 |
| C | 18.427405 | 7.999965 | 18.735035 |
| C | 12.881131 | 4.824764 | 21.061424 |
| C | 14.459397 | 6.209992 | 19.716313 |
| C | 12.542321 | 7.309238 | 20.902743 |
| C | 18.809113 | 5.990342 | 17.298171 |
| H | 12.736551 | 5.975447 | 18.435747 |
| H | 16.472993 | 6.195693 | 16.392759 |
| H | 16.360586 | 6.430636 | 20.677532 |
| H | 13.741462 | 6.345039 | 23.124272 |
| H | 15.146153 | 5.591555 | 22.388661 |
| H | 14.919353 | 7.338034 | 22.268111 |
| H | 19.837458 | 5.826895 | 19.744315 |
| H | 11.926267 | 7.312415 | 21.800808 |
| H | 19.891080 | 6.089045 | 17.402237 |

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| H | 12.250778 | 4.779881 | 21.952935 |
| H | 13.614160 | 4.015672 | 21.121004 |
| H | 12.251374 | 4.646819 | 20.191163 |
| H | 17.997041 | 8.385446 | 19.650775 |
| H | 18.587278 | 4.942136 | 17.103743 |
| H | 11.878405 | 7.182929 | 20.051349 |
| H | 13.023129 | 8.279791 | 20.819133 |
| H | 18.516179 | 6.557540 | 16.416392 |
| H | 18.417078 | 6.123999 | 20.727976 |
| H | 18.013525 | 8.563390 | 17.903700 |
| H | 19.507983 | 8.180889 | 18.765620 |
| H | 18.499100 | 4.677801 | 19.722867 |
| C | 15.358058 | 3.655612 | 10.017334 |
| C | 13.914442 | 3.642504 | 12.414026 |
| C | 16.011846 | 3.848054 | 13.778004 |
| C | 15.381095 | 3.484022 | 7.478444 |
| C | 17.249515 | 2.533726 | 8.813426 |
| C | 15.307217 | 3.765238 | 12.441632 |
| C | 13.961907 | 3.549163 | 10.014950 |
| C | 13.218551 | 3.543602 | 11.207935 |
| C | 11.058588 | 4.368384 | 12.238663 |
| C | 16.212431 | 3.666138 | 8.746300 |
| C | 11.694105 | 3.391475 | 11.232362 |
| C | 16.011449 | 3.775566 | 11.245271 |
| C | 16.938112 | 5.022370 | 8.656533 |
| C | 11.353905 | 1.955207 | 11.664116 |
| C | 11.065539 | 3.654222 | 9.863817 |
| H | 13.445748 | 3.467737 | 9.071407 |
| H | 13.376834 | 3.623637 | 13.363330 |
| H | 17.092423 | 3.883802 | 11.282211 |
| H | 16.036472 | 3.480050 | 6.603814 |

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| H | 15.378116 | 4.481784 | 14.411734 |
| H | 9.979600 | 3.586698 | 9.940277 |
| H | 14.835147 | 2.537499 | 7.484402 |
| H | 14.655216 | 4.285766 | 7.343198 |
| H | 17.866363 | 2.522207 | 7.914369 |
| H | 17.538675 | 5.076786 | 7.752113 |
| H | 16.217396 | 5.841790 | 8.631113 |
| H | 17.913034 | 2.625479 | 9.672963 |
| H | 9.972649 | 4.252005 | 12.224960 |
| H | 17.599049 | 5.187406 | 9.507530 |
| H | 16.759968 | 1.561981 | 8.887305 |
| H | 11.309617 | 4.649203 | 9.496408 |
| H | 10.269554 | 1.811223 | 11.703439 |
| H | 11.384092 | 2.929335 | 9.111921 |
| H | 11.765402 | 1.737543 | 12.646983 |
| H | 11.293332 | 5.397325 | 11.979492 |
| H | 11.388064 | 4.200369 | 13.258271 |
| H | 11.761231 | 1.232307 | 10.960679 |
| C | 19.772516 | 4.501842 | 13.585562 |
| C | 17.375824 | 5.945458 | 13.572454 |
| C | 22.311406 | 4.478805 | 13.413972 |
| C | 20.976424 | 2.610385 | 12.463676 |
| C | 17.348218 | 4.552683 | 13.695188 |
| C | 19.774900 | 5.897993 | 13.479113 |
| C | 18.581915 | 6.641349 | 13.473552 |
| C | 17.551187 | 8.801312 | 14.298334 |
| C | 21.043550 | 3.647469 | 13.596088 |
| C | 18.557488 | 8.165795 | 13.321425 |
| C | 18.544579 | 3.848451 | 13.705516 |
| C | 21.133317 | 2.921788 | 14.952320 |
| C | 18.125734 | 8.505995 | 11.885157 |

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| C | 19.926033 | 8.794361 | 13.584172 |
| H | 20.718443 | 6.414152 | 13.397687 |
| H | 16.426520 | 6.483066 | 13.553587 |
| H | 18.507639 | 2.767477 | 13.813752 |
| H | 23.186036 | 3.823428 | 13.410000 |
| H | 19.849573 | 9.880300 | 13.516648 |
| H | 22.305448 | 5.024753 | 12.467449 |
| H | 22.446652 | 5.204684 | 14.215716 |
| H | 21.875481 | 1.993537 | 12.452157 |
| H | 22.037737 | 2.321225 | 15.006736 |
| H | 21.158737 | 3.642504 | 15.771740 |
| H | 20.116887 | 1.946866 | 12.555429 |
| H | 17.564890 | 9.887251 | 14.181955 |
| H | 20.282320 | 2.260851 | 15.117356 |
| H | 20.902545 | 3.099932 | 11.491931 |
| H | 20.293442 | 8.550283 | 14.579153 |
| H | 18.086411 | 9.590346 | 11.741173 |
| H | 20.677929 | 8.475808 | 12.859285 |
| H | 17.142867 | 8.094498 | 11.667493 |
| H | 17.810358 | 8.566568 | 15.327275 |
| H | 16.531579 | 8.471836 | 14.130319 |
| H | 18.829171 | 8.098669 | 11.162257 |
| C | 16.204288 | 0.087384 | 14.431792 |
| C | 16.217396 | 2.484076 | 15.875408 |
| C | 16.375878 | -2.451506 | 14.408755 |
| C | 17.326174 | -1.116524 | 12.540335 |
| C | 16.094662 | 2.511682 | 14.482633 |
| C | 16.310737 | 0.085000 | 15.827943 |
| C | 16.316298 | 1.277985 | 16.571299 |
| C | 15.491516 | 2.308713 | 18.731262 |
| C | 16.193762 | -1.183650 | 13.577419 |

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C       16.468425    1.302412   18.095745
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C       14.837530   -1.273417   12.851738
C       17.904693    1.734166   18.435945
C       16.205678   -0.066133   18.724311
H       16.392163   -0.858543   16.344102
H       16.236263    3.433380   16.413016
H       15.976098    1.352261   12.697427
H       16.379850   -3.326136   13.753378
H       16.273202    0.010327   19.810250
H       17.322401   -2.445548   14.954703
H       15.574134   -2.586752   15.134634
H       17.337693   -2.015581   11.923487
H       14.783114   -2.177837   12.251175
H       14.018110   -1.298837   13.572454
H       17.234421   -0.256987   11.876816
H       15.607895    2.295010   19.817201
H       14.672494   -0.422420   12.190801
H       18.297919   -1.042645   13.029882
H       15.210697   -0.433542   18.480233
H       18.048677    1.773489   19.520296
H       16.930565   -0.818029   18.405758
H       18.122357    2.717033   18.024448
H       14.462575    2.049542   18.496518
H       15.659531    3.328321   18.401786
H       18.627593    1.030729   18.028619

case_studies/thiocyanate_dimer.xyz

102
symmetry c1
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C 5.420456274 -1.147664630 -1.951469698
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H 7.348641075 -2.285122601 -4.325555859
C 8.076081540 -1.983005623 -2.458502651
H 8.945074028 -2.268815676 -2.623845341
C 7.701796088 -1.526787623 -1.191312094
C 8.479867672 -1.391402107 0.048219030
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C 10.292005586 -1.458096482 1.625161947
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H 5.558451689 -1.178018628
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H 1.339419977 1.423770750
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C 0.198004123 0.442439628
0.373921473
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C 0.825422520 5.389406504
0.517709550
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C 3.586988814 1.019546821
0.804566208
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C       -3.525372115     -2.978897619
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H       -6.319058379     -2.163764607
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case_studies/propane_dimer.xyz

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22
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  H          0.956045646235
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  C          0.019262196246
-1.397545158303     -1.872184732721
  H         -0.789703692469
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0.585132167386 -1.665104906892
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-0.001774448298 0.240794173857
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H -0.886043707550
-1.922987439962 -1.567613056262
H 0.041927317395
-1.377168263755 -2.961189731795
H 0.871606546773
-0.543623848232 0.646060158414
H -0.887698654161
-0.491623546811 0.602795509296
H 0.034878564125
1.007867541367 0.649224668681
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0.672234677120 -0.207675832879
H -2.870478741685
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C -3.801700793432
-0.737812172618 -0.787760055335
H -4.629522554326
1.251521102137 -0.560578067263
H -3.806348938688
0.658217113388 0.881218051938
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  H        -4.619748346631
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case_studies/propane.xyz

11
Coordinates from ORCA-job
/scratch/83611013.tmpdir/opt1_pbe_tzvp
  C   1.27016012179937      0.26370964585672
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  H   1.32024256420662      0.92482348609988
    -0.87451740200098
  H   1.31770667664957      0.90313415882563
     0.89971134653229
  H   2.16968017320850     -0.36896485137559
    -0.00186107383150
  C   -0.00962085756527
-0.57305238174367     -0.00747307876224
  H   -0.01506345897941
-1.24785545023777      0.86462412080494
  H   -0.01241528033670
-1.22677873884343     -0.89548308330514
  C   -1.27842351962755
0.28006456528272      0.00092417824049
  H   -2.18613127081264
-0.34075320568026     -0.00945612766180
  H   -1.32079633997007
```

```
0.9190846185006 0.8966035243209
  H -1.3166634495724
0.9426677493151 -0.8776525379051

case_studies/perfluoropropane_dimer.xyz

22
final.xyz
  C -0.4020772248864
-0.8884281040264 -2.3701000424644
  F -1.4164906224214
-1.0385027362884 -3.2140745214584
  F 0.4550674128644
-0.0133859534974 -2.8844857153154
  F 0.2075625738934
-2.0578189216004 -2.2181528005644
  C -0.9503838713604
-0.3831505436544 -1.0148460552534
  F -1.5820123935174
0.7799302439734 -1.2311162387834
  F -1.8285207368164
-1.2873847796434 -0.5562498582074
  C 0.1136989295684
-0.1533867632784 0.0833593027694
  F 1.0076004139644
0.7464087208764 -0.3134313369964
  F 0.7392630173314
-1.2874914654914 0.3728672647364
  F -0.4909735104874
0.2957788502984 1.1771638090044
  C 3.9605037819114
```

```
-0.548508195303     -2.096352930498
  F          3.339997946503
0.592529012702     -2.368938175324
  C          5.026833192507
-0.339941766151     -0.996133378400
  F          3.063001575698
-1.449870643039     -1.711345848109
  F          4.561884690141
-0.984943613322     -3.197098456295
  F          5.909339501891
0.566109130318     -1.442496973192
  F          5.652258171261
-1.509497397756     -0.797229027795
  C          4.482886534458
0.148930820782      0.366795857734
  F          3.876383397746
1.322062947578      0.231796748124
  F          5.499772616500
0.284710746957      1.210294748221
  F          3.624055957254
-0.729929181437      0.871348215066

elements/K_F.xyz

2
Coordinates from ORCA-job
/scratch/86428463.tmpdir/opt1_tpss_qzvp
  K   0.0825170705657      0.0000000000000
     0.0000000000000
  F   2.2574829294342      0.0000000000000
     0.0000000000000
```

elements/Tl_H.xyz

```
4
Coordinates from ORCA-job
/scratch/86428394.tmpdir/opt1_tpss_qzvp
  Tl  -0.00007756776438
0.0000376716791      0.0226901012766 7
  H   1.74719931419955     -0.0004264359317 9
    -0.00641567020342
  H   -0.8739292582232 5
1.51304402919727     -0.00642915497065
  H   -0.87319248821193
-1.51262136043341      0.08090472389728
```

elements/Al_H.xyz

```
4
Coordinates from ORCA-job
/scratch/86428324.tmpdir/opt1_tpss_qzvp
  Al  -0.0000062105586 0
-0.00001469835021      0.02240819395157
  H   1.58300377715232     -0.0003561938564 2
    -0.00396726475120
  H   -0.7918115134623 4
1.37074115259734     -0.00396805291676
  H   -0.7911860531313 8
-1.37037026039071      0.07515212371641
```

elements/Ca_F.xyz

```
3
Coordinates from ORCA-job
/scratch/86428443.tmpdir/opt1_tpss_qzvp
  Ca  -0.0113400993151 
3
0.0000000000001     -0.4087578014022
  F   1.8755092026524     -0.0000000000002
     0.2254170051824
  F   -1.8641691033373
0.0000000000012      0.3183407962245

elements/At_H.xyz

2
Coordinates from ORCA-job
/scratch/86428327.tmpdir/opt1_tpss_qzvp
  At  0.0725902183205      0.0000000000000
     0.0000000000000
  H   1.7799097816795      0.0000000000000
     0.0000000000000

elements/O_F.xyz

3
Coordinates from ORCA-job
/scratch/86428476.tmpdir/opt1_tpss_qzvp
  O   -0.0144445267845
0.0000000000000     -0.5528409816100
  F   1.1315175358168      0.0000000000000
     0.2912393061390
  F   -1.1170730090323
0.0000000000000      0.3471016754710
```

```
elements/Se_F.xyz

3
Coordinates from ORCA-job
/scratch/86428494.tmpdir/opt1_tpss_qzvp
  Se  -0.0192192321543 7
-0.0000000000004     -0.7354070778493 9
  F   1.3240851710760 5      0.0000000000000 2
     0.3911137803492 3
  F   -1.3048659389270 8
-0.0000000000024 1      0.4562932970780 8

elements/Si_F.xyz

5
Coordinates from ORCA-job
/scratch/86428495.tmpdir/opt1_tpss_qzvp
  Si  -0.0000024128649 7
0.0000036808245 2      0.0232085689632 8
  F   0.9183469327785 4     -0.8989184976602 1
    -0.8854417135411 5
  F   -0.8989188681477 7
0.9183770408031 4     -0.8853968667613
  F   -0.9182721124279 3
-0.9182756379929 1      0.9123714948776 0
  F   0.8988464606621 3      0.8988134140254 6
     0.9512613363763 9

elements/F_F.xyz
```

```
2
Coordinates from ORCA-job
/scratch/86428452.tmpdir/opt1_tpss_qzvp
  F   0.1072922440477900      0.0000000000000000
     0.0000000000000000
  F   1.5227077559522100      0.0000000000000000
     0.0000000000000000

elements/Br_F.xyz

2
Coordinates from ORCA-job
/scratch/86428438.tmpdir/opt1_tpss_qzvp
  Br  0.2053607993329400      0.0000000000000000
     0.0000000000000000
  F   1.9846392006670600      0.0000000000000000
     0.0000000000000000

elements/Pb_F.xyz

5
Coordinates from ORCA-job
/scratch/86428479.tmpdir/opt1_tpss_qzvp
  Pb  0.0000074514201400      0.0000178710983000
     0.0249759644357000
  F   1.1678563668085300     -1.1431154046964400
    -1.1305459269995600
  F   -1.1431206549373000
1.1678575968139900     -1.1305592129046000
  F   -1.1678611691715500
-1.1678681297689200      1.1555329342142400
```

```
  F   1.14311800588018      1.14310806655306
     1.20509624125421

elements/Na_F.xyz

2
Coordinates from ORCA-job
/scratch/86428471.tmpdir/opt1_tpss_qzvp
  Na  0.15178284038970      0.00000000000000
     0.00000000000000
  F   2.09821715961030      0.00000000000000
     0.00000000000000

elements/H_H.xyz

2
Coordinates from ORCA-job
/scratch/86428346.tmpdir/opt1_tpss_qzvp
  H   0.20639864730058      0.00000000000000
     0.00000000000000
  H   0.94860135269942      0.00000000000000
     0.00000000000000

elements/Te_F.xyz

3
Coordinates from ORCA-job
/scratch/86459232.tmpdir/opt1_tpss_qzvp
  Te  -0.0000554920771
0.00000701206444     -0.00000031120471
  F   0.00000277460732     -0.00000350603685
```

```
    -1.99465341539385
  F   0.00000277460040      -0.00000350602759
     1.99465372659856

elements/Cl_H.xyz

2
Coordinates from ORCA-job
/scratch/86428337.tmpdir/opt1_tpss_qzvp
  Cl  0.13093728158198       0.00000000000000
     0.00000000000000
  H   1.41406271841802       0.00000000000000
     0.00000000000000

elements/N_H.xyz

4
Coordinates from ORCA-job
/scratch/86428364.tmpdir/opt1_tpss_qzvp
  N   -0.00487593791446
-0.00844564122254     -0.27659569748305
  H   0.94201063253445       0.00259407260701
     0.09895740111596
  H   -0.46875884248703
0.81710272288809      0.09895814058227
  H   -0.46837585213282
-0.81125115427252      0.14580515578492

elements/P_F.xyz

4
```

```
Coordinates from ORCA-job
/scratch/86428478.tmpdir/opt1_tpss_qzvp
  P   -0.0097132794349
-0.0168867656826     -0.5609121706935
  F   1.3839201979004      0.0052831758295
     0.2012794213026
  F   -0.6874034816535
1.2012677614125      0.2012451944055
  F   -0.6868034368122
-1.1896641715600      0.2698875549865

elements/Sn_F.xyz

5
Coordinates from ORCA-job
/scratch/86428496.tmpdir/opt1_tpss_qzvp
  Sn  0.0000080855023      0.0000110435360
     0.0248440339009
  F   1.1059748659078     -1.0825439617532
    -1.0693965862381
  F   -1.0825439189334
1.1059768998710     -1.0694002177095
  F   -1.1059334351554
-1.1059369084348      1.0955124792093
  F   1.0824944026786      1.0824929267809
     1.1424402908373

elements/Sr_F.xyz

3
Coordinates from ORCA-job
```

```
/scratch/86428498.tmpdir/opt1_tpss_qzvp
  Sr  -0.01583561227226
-0.00000000000001     -0.58968938511861
  F   1.90013822893262      0.00000000000001
     0.31770556843978
  F   -1.88430261666034
-0.00000000000009      0.41148381667647

elements/As_H.xyz

4
Coordinates from ORCA-job
/scratch/86428326.tmpdir/opt1_tpss_qzvp
  As  -0.01043558254305
-0.01833197960467     -0.61602623344309
  H   1.26829327595492      0.00588210412421
     0.21344781304883
  H   -0.6291587120708 3
1.10128545861247      0.21320812750264
  H   -0.62869898134095
-1.08883558313246      0.27599529289162

elements/Bi_F.xyz

4
Coordinates from ORCA-job
/scratch/86428437.tmpdir/opt1_tpss_qzvp
  Bi  -0.01254165398709
-0.02200392631636     -0.74707359817293
  F   1.72337044376026      0.00628519343786
     0.26204745002013
```

```
  F   -0.8563215780021
1.4956131667948      0.2621321808514
  F   -0.8545072117741
-1.4798944339215      0.3478939673041

elements/Rb_F.xyz

2
Coordinates from ORCA-job
/scratch/86428484.tmpdir/opt1_tpss_qzvp
  Rb  0.0321445784517      0.0000000000000
     0.0000000000000
  F   2.3678554215482      0.0000000000000
     0.0000000000000

elements/In_H.xyz

4
Coordinates from ORCA-job
/scratch/86428353.tmpdir/opt1_tpss_qzvp
  In  0.0000151739740      0.0000240970853
     0.0230595741406
  H   1.7279213921119     -0.0004508414566
    -0.0057227897656
  H   -0.8643517742842
1.4961942973356     -0.0057239341417
  H   -0.8635847918018
-1.4957675529643      0.0806371497667

elements/I_H.xyz
```

```
2
Coordinates from ORCA-job
/scratch/86428351.tmpdir/opt1_tpss_qzvp
  I   0.0845294052694      0.0000000000000
     0.0000000000000
  H   1.7004705947305      0.0000000000000
     0.0000000000000

elements/Li_F.xyz

2
Coordinates from ORCA-job
/scratch/86428465.tmpdir/opt1_tpss_qzvp
  Li  0.3126271851397      0.0000000000000
     0.0000000000000
  F   1.8873728148602      0.0000000000000
     0.0000000000000

elements/Sn_H.xyz

5
Coordinates from ORCA-job
/scratch/86428387.tmpdir/opt1_tpss_qzvp
  Sn  -0.0000090688289
-0.0000070652294      0.0186023096834
  H   0.9966685673320     -0.9755251257291
    -0.9673861584495
  H   -0.9755262232017
0.9966682061478     -0.9673882501134
  H   -0.9965529092033
-0.9965536292727      0.9834627741018
```

```
  H   0.97541963390192      0.97541761408347
     1.02570932477763

elements/O_H.xyz

3
Coordinates from ORCA-job
/scratch/86428369.tmpdir/opt1_tpss_qzvp
  O   -0.00982898107828
0.00000000000000     -0.37432721246314
  H   0.76815350637231      0.00000000000000
     0.20026197531561
  H   -0.75832452529401
0.00000000000000      0.23819023714754

elements/B_F.xyz

4
Coordinates from ORCA-job
/scratch/86428434.tmpdir/opt1_tpss_qzvp
  B   -0.00001370565499
-0.00000443498722      0.02563353081090
  F   1.32091186769985     -0.00030524003044
     0.00361590906066
  F   -0.66071472798890
1.14380616357318      0.00361433134198
  F   -0.66018343405597
-1.14349648855551      0.06963622878646

elements/Ga_F.xyz
```

```
4
Coordinates from ORCA-job
/scratch/86428454.tmpdir/opt1_tpss_qzvp
  Ga  -0.00013195802404
-0.00001214143304      0.02907581612981
  F   1.73567384869736     -0.00035390058808
     0.00022375576099
  F   -0.86808099115294
1.50313865095697      0.00021635995799
  F   -0.86746089952038
-1.50277260893584      0.08698406815120

elements/Ba_H.xyz

3
Coordinates from ORCA-job
/scratch/86428330.tmpdir/opt1_tpss_qzvp
  Ba  -0.02017387721264
0.00000000000000     -0.77512603640658
  H   1.93382997237172      0.00000000000000
     0.39468452302140
  H   -1.91365609515907
0.00000000000000      0.49031651338533

elements/Ge_F.xyz

5
Coordinates from ORCA-job
/scratch/86428455.tmpdir/opt1_tpss_qzvp
  Ge  -0.00000045273429
0.00000465715393      0.02343720447333
```

```
  F   0.9954047464380     -0.9743035074596
    -0.9613368243688
  F   -0.9743039028138
0.9954043910909     -0.9613404075582
  F   -0.9953565384815
-0.9953589576756      0.9870089684924
  F   0.9742561475916      0.9742534168904
     1.0292310589613

elements/Be_H.xyz

3
Coordinates from ORCA-job
/scratch/86428331.tmpdir/opt1_tpss_qzvp
  Be  -0.0000037347024
0.0000000016945      0.0272114060180
  H   1.3310990806101     -0.0000000008473
    -0.0058207739721
  H   -1.3310953459076
-0.0000000008472      0.0607343679541

elements/H_F.xyz

2
Coordinates from ORCA-job
/scratch/86428456.tmpdir/opt1_tpss_qzvp
  H   0.3058603894644      0.0000000000000
     0.0000000000000
  F   1.2341396105356      0.0000000000000
     0.0000000000000
```

elements/Tl_F.xyz

4
Coordinates from ORCA-job
/scratch/86428503.tmpdir/opt1_tpss_qzvp
  Tl  -0.00433069915643
0.00039885036726      0.03054023977092
  F   2.01187356671712     -0.00085951743271
     0.00946042442991
  F   -1.00434608087320
1.74947774131149     -0.00950222150867
  F   -1.00319678668767
-1.74901707424521      0.09050155729864

elements/S_H.xyz

3
Coordinates from ORCA-job
/scratch/86428382.tmpdir/opt1_tpss_qzvp
  S   -0.01539592975396
0.00000000000000     -0.59395189936996
  H   0.97637959783316      0.00000000000000
     0.31307911626635
  H   -0.96098366807920
0.00000000000000      0.36112278310362

elements/Al_F.xyz

4
Coordinates from ORCA-job
/scratch/86428429.tmpdir/opt1_tpss_qzvp

```
  Al  -0.0002419123045
-0.0001243550813      0.0299563394399
  F   1.6416160026433     -0.0001402097627
     0.0024945263507
  F   -0.8208532866990
1.4218190511074      0.0024865833821
  F   -0.8205385247139
-1.4215544862633      0.0845625508270

elements/Mg_H.xyz

3
Coordinates from ORCA-job
/scratch/86428360.tmpdir/opt1_tpss_qzvp
  Mg  -0.0000000702370
0.0000002539709      0.0299977618659
  H   1.7063591698309     -0.0000001269855
    -0.0126588588434
  H   -1.7063591628072
-0.0000001269855      0.0726590826568

elements/Cs_H.xyz

2
Coordinates from ORCA-job
/scratch/86428340.tmpdir/opt1_tpss_qzvp
  Cs  -0.3120423678993
0.0000000000000      0.0000000000000
  H   2.1795423678993      0.0000000000000
     0.0000000000000
```

```
elements/N_F.xyz

4
Coordinates from ORCA-job
/scratch/86428470.tmpdir/opt1_tpss_qzvp
  N   -0.0077684676108
-0.0134565821187     -0.4455743079648
2
  F   1.2551473546681      0.0042067489660
7     0.1575843001120
2
  F   -0.6239318761793
1.0891306980523      0.1575721084428
5
  F   -0.6234486317276
-1.0798808608066      0.2199178994093
7

elements/At_F.xyz

2
Coordinates from ORCA-job
/scratch/86428432.tmpdir/opt1_tpss_qzvp
  At  0.2264568794875      0.0000000000000
0     0.0000000000000
  F   2.2435431205124      0.0000000000000
0     0.0000000000000

elements/Ca_H.xyz

3
Coordinates from ORCA-job
/scratch/86428335.tmpdir/opt1_tpss_qzvp
  Ca  -0.0128039552898
5.0000000000000     -0.4801331701296
0
```

```
  H   1.85971228855248      0.00000000000000
     0.24450067276661
  H   -1.84690833326263
0.00000000000000      0.33688249736301

elements/P_H.xyz

4
Coordinates from ORCA-job
/scratch/86428371.tmpdir/opt1_tpss_qzvp
  P   -0.00957915163760
-0.01656289960595     -0.55634909312107
  H   1.19494695515796      0.00523508150574
     0.19359956809988
  H   -0.59293178346096
1.03750582283956      0.19358266664195
  H   -0.59243602005886
-1.02617800473917      0.25279185838030

elements/C_F.xyz

5
Coordinates from ORCA-job
/scratch/86428439.tmpdir/opt1_tpss_qzvp
  C   -0.00000030808796
0.00000048407522      0.01900141315044
  F   0.77896407789065     -0.76244314797662
    -0.75163765525237
  F   -0.76245950015670
0.77897432605185     -0.75160996977082
  F   -0.77887814885856
```

```
-0.7788945353265       0.7731044527289
  F   0.7623738792125       0.7623628731761
     0.8061417591438

elements/Se_H.xyz

3
Coordinates from ORCA-job
/scratch/86428385.tmpdir/opt1_tpss_qzvp
  Se  -0.0170293007020
0.0000000000000     -0.6589035398385
  H   1.0579604948173       0.0000000000000
     0.3454320217245
  H   -1.0409311941153
0.0000000000000       0.3974715181139

elements/Si_H.xyz

5
Coordinates from ORCA-job
/scratch/86428386.tmpdir/opt1_tpss_qzvp
  Si  0.0000014968411       0.0000015247578
     0.0173981852102
  H   0.8644511464501     -0.8461245859396
    -0.8377586074204
  H   -0.8461245836969
0.8644511685246     -0.8377586492459
  H   -0.8643511871219
-0.8643512255703       0.8542282011512
  H   0.8460231275274       0.8460231182275
     0.8908908703048
```

```
elements/I_F.xyz

2
Coordinates from ORCA-job
/scratch/86428460.tmpdir/opt1_tpss_qzvp
  I   0.22737318475076      0.00000000000000
     0.00000000000000
  F   2.15262681524924      0.00000000000000
     0.00000000000000

elements/Br_H.xyz

2
Coordinates from ORCA-job
/scratch/86428333.tmpdir/opt1_tpss_qzvp
  Br  0.10831659749825      0.00000000000000
     0.00000000000000
  H   1.53418340250175      0.00000000000000
     0.00000000000000

elements/Pb_H.xyz

5
Coordinates from ORCA-job
/scratch/86428372.tmpdir/opt1_tpss_qzvp
  Pb  0.00000484761721     -0.00000528348006
     0.01866868772177
  H   1.02769652578010     -1.00590738378328
    -0.99800884968403
  H   -1.00590631227898
```

```
1.0276954689704 3     -0.9980015265889
  H   -1.0275771900410
7
-1.0275711079109 7      1.0135691720427
4
  H   1.0057821289227 6      1.0057883062038
8    1.0571475165085 1

elements/Na_H.xyz

2
Coordinates from ORCA-job
/scratch/86428365.tmpdir/opt1_tpss_qzvp
  Na  -0.1048309718255
2
0.0000000000000 0      0.0000000000000
0
  H   1.7923309718255 0      0.0000000000000
0    0.0000000000000 0

elements/Cl_F.xyz

2
Coordinates from ORCA-job
/scratch/86428445.tmpdir/opt1_tpss_qzvp
  Cl  0.2054516673745 2      0.0000000000000
0    0.0000000000000 0
  F   1.8545483326254 8      0.0000000000000
0    0.0000000000000 0

elements/Po_F.xyz

3
Coordinates from ORCA-job
/scratch/86428481.tmpdir/opt1_tpss_qzvp
```

```
  Po  0.0000057968742     -0.0000062567450
     0.04166357955642
  F   2.09693798260921      0.0000031283706
    -0.01075524112683
  F   -2.09693856229676
0.0000031283726      0.09409166157557

elements/K_H.xyz

2
Coordinates from ORCA-job
/scratch/86428356.tmpdir/opt1_tpss_qzvp
  K   -0.24516460245707
0.00000000000000      0.00000000000000
  H   2.00016460245707      0.00000000000000
     0.00000000000000

elements/Te_H.xyz

3
Coordinates from ORCA-job
/scratch/86428391.tmpdir/opt1_tpss_qzvp
  Te  -0.0194731063064
0.00000000000000     -0.75231486037060
  H   1.18448577368559      0.00000000000000
     0.39233354823081
  H   -1.16503846305495
0.00000000000000      0.45073131213978

elements/B_H.xyz
```

```
4
Coordinates from ORCA-job
/scratch/86428329.tmpdir/opt1_tpss_qzvp
  B   0.00000087681056     -0.00000802012387
     0.01902613277768
  H   1.19123503148284     -0.00028132906697
    -0.00056304026285
  H   -0.5958639085507 2
1.03148542734234     -0.00056283036653
  H   -0.59537199974268
-1.03119607815150      0.05897473785170

elements/S_F.xyz

3
Coordinates from ORCA-job
/scratch/86428490.tmpdir/opt1_tpss_qzvp
  S   0.00000000657417      0.00000000839060
     0.03566839328638
  F   1.69748112855208     -0.00000000419530
    -0.00677121947624
  F   -1.69748113512624
-0.00000000419530      0.07810282618984

elements/As_F.xyz

4
Coordinates from ORCA-job
/scratch/86428431.tmpdir/opt1_tpss_qzvp
  As  -0.01101067094544
-0.01904846235972     -0.63595146536974
```

```
  F   1.49499088779591      0.00597276204605
     0.22578241107969
  F   -0.74231608895333
1.29787813190825      0.22579652392914
  F   -0.74166412789564
-1.28480243159532      0.29987253036068

elements/Sr_H.xyz

3
Coordinates from ORCA-job
/scratch/86428388.tmpdir/opt1_tpss_qzvp
  Sr  -0.01705047889398
0.00000000000000     -0.65078953318874
  H   1.90291152688811      0.00000000000000
     0.33061093804078
  H   -1.88586104799413
0.00000000000000      0.42480359514801

elements/Sb_F.xyz

4
Coordinates from ORCA-job
/scratch/86428492.tmpdir/opt1_tpss_qzvp
  Sb  -0.01107418481534
-0.02144640307243     -0.71633750145368
  F   1.62832183911475      0.00537572401596
     0.25489834071151
  F   -0.80838421407892
1.41393610485874      0.25134809020670
  F   -0.80886344021929
```

```
-1.3978654258024      0.3330910705290

elements/In_F.xyz

4
Coordinates from ORCA-job
/scratch/86428461.tmpdir/opt1_tpss_qzvp
  In  -0.0003140010264
7
-0.0001537045762      0.0309536183733
5
  F   1.9334176749693     -0.0001320352522
3
    -0.0015343119201
  F   -0.9667106419148
9
1.6746014253262     -0.0015456871540
2
  F   -0.9663930320279
4
-1.6743156854977      0.0951263807008

elements/F_H.xyz

2
Coordinates from ORCA-job
/scratch/86428342.tmpdir/opt1_tpss_qzvp
  F   0.1471103905204      0.0000000000000
0
    0.0000000000000
  H   1.0753896094795      0.0000000000000
0
    0.0000000000000

elements/Po_H.xyz

3
Coordinates from ORCA-job
/scratch/86428374.tmpdir/opt1_tpss_qzvp
```

```
  Po  -0.0204702831079
3 0.0000000000000     -0.7986711342587
9
  H   1.2409757515185      0.0000000000000
     0.4158096219338
  H   -1.2205054684106
6 0.0000000000000      0.4766115123249
5

elements/Bi_H.xyz

4
Coordinates from ORCA-job
/scratch/86428332.tmpdir/opt1_tpss_qzvp
  Bi  -0.0129775030630
0 -0.0223691509536     -0.7561344963927
9
  H   1.4719481927750      0.0070992562990
4     0.2589144677973
8
  H   -0.7297930058604
7 1.2783422629183      0.2589977980733
0
  H   -0.7291776838507
8 -1.2630723682645      0.3319722305128
4

elements/Rb_H.xyz

2
Coordinates from ORCA-job
/scratch/86428376.tmpdir/opt1_tpss_qzvp
  Rb  -0.3036049224619
7 0.0000000000000      0.0000000000000
0
  H   2.1036049224619      0.0000000000000
7     0.0000000000000
```

```
elements/Li_H.xyz

2
Coordinates from ORCA-job
/scratch/86428358.tmpdir/opt1_tpss_qzvp
  Li  0.0265812955141      0.0000000000000
     0.0000000000000
  H   1.6234198704859      0.0000000000000
     0.0000000000000

elements/Ba_F.xyz

3
Coordinates from ORCA-job
/scratch/86428435.tmpdir/opt1_tpss_qzvp
  Ba  -0.0179386121409
-0.0000000000006     -0.6865153006288
  F   1.9351148382545      0.0000000000011
     0.3686343131484
  F   -1.9171762261409
-0.0000000000102      0.4643809874792

elements/C_H.xyz

5
Coordinates from ORCA-job
/scratch/86428334.tmpdir/opt1_tpss_qzvp
  C   -0.0000030419734
0.0000043084205      0.0142502151029
  H   0.6368560184341     -0.6232922186196
    -0.6157546152075
```

```
  H   -0.62330741878257
0.63684611008598     -0.61575092610160
  H   -0.63677084095241
-0.63678622407565      0.63070124065426
  H   0.62322254549813      0.62323190176724
     0.65780408555191

elements/Be_F.xyz

3
Coordinates from ORCA-job
/scratch/86428436.tmpdir/opt1_tpss_qzvp
  Be  -0.00000371920272
-0.00000001374063      0.03622764031073
  F   1.38667813686688      0.00000000687028
     0.00196865707350
  F   -1.38667441766416
0.00000000687035      0.07130370261577

elements/Ga_H.xyz

4
Coordinates from ORCA-job
/scratch/86428344.tmpdir/opt1_tpss_qzvp
  Ga  0.00002706286897      0.00003968577403
     0.02174599501164
  H   1.56389521041001     -0.00043335033397
    -0.00417760298463
  H   -0.78232499224752
1.35415098213630     -0.00417832668114
  H   -0.78159728103149
```

```
-1.3537573175763 0.0739849346540

elements/Sb_H.xyz

4
Coordinates from ORCA-job
/scratch/86428383.tmpdir/opt1_tpss_qzvp
  Sb  -0.0120307488928
-0.0209399244619 -0.7048016972038
  H   1.4155163305762 0.0067358302173
    0.2423845337115
  H   -0.7019633277991
1.2291974285865 0.2422940492481
  H   -0.7015222538852
-1.2149933343421 0.3123731142423

elements/Mg_F.xyz

3
Coordinates from ORCA-job
/scratch/86428467.tmpdir/opt1_tpss_qzvp
  Mg  0.0000205673489 0.0000186611416
    0.0399931187500
  F   1.7548665484358 -0.0000453605224
   -0.0033173745912
  F   -1.7548871157841
0.0000266993815 0.0833242558391

elements/Ge_H.xyz

5
```

```
Coordinates from ORCA-job
/scratch/86428345.tmpdir/opt1_tpss_qzvp
  Ge  0.0000030474993      0.0000233633781
     0.01755033721195
  H   0.89453489244184     -0.87557084602185
    -0.86740094737958
  H   -0.87557082376020
0.89453539186378     -0.86740245456243
  H   -0.89443387723140
-0.89443537575856      0.88353459044851
  H   0.87546950379984      0.87546849357881
     0.92146847428155

elements/Cs_F.xyz

2
Coordinates from ORCA-job
/scratch/86428448.tmpdir/opt1_tpss_qzvp
  Cs  0.06073865534825      0.00000000000000
     0.00000000000000
  F   2.42926134465175      0.00000000000000
     0.00000000000000

substituents/17.xyz

  5
         -8.45522566
 H         -2.9273540812       -0.0045307106
       0.0000131589
 C         -1.8788069112        0.0078776105
       0.0000048200
```

```
 C          -0.6794070612        -0.0229637682
      -0.0000107689
 S           1.0134388787         0.0460714136
       0.0000016729
 H           1.1770391401        -1.2811619963
       0.0000045201

substituents/2.xyz

  10
        -11.54622935
 H           2.8416662677         0.6435334804
       0.0000464929
 C           1.8597775892         0.2749192583
      -0.0000061015
 C           0.7445125447        -0.1580658941
      -0.0000018952
 C          -0.6179041944        -0.6522890532
       0.0000064209
 H          -0.7661931488        -1.2772461480
       0.8859021791
 C          -1.6246652075         0.4985170173
       0.0000014274
 H          -2.6405726199         0.1092687960
      -0.0002502503
 H          -1.4895141064         1.1209186883
      -0.8818889270
 H          -1.4897976849         1.1207551180
       0.8820707909
 H          -0.7661628846        -1.2772754098
      -0.8858785177
```

substituents/5.xyz

```
  11
        -13.66238376
 H          -3.1942923204        -0.0000319804
      -0.5387089664
 C          -2.1948021701        -0.0000015188
      -0.2216631076
 C          -1.0573755696         0.0000100732
       0.1545299210
 C           0.3056341209         0.0000141953
       0.5806906494
 C           1.3291430891        -0.7471003129
      -0.2341884154
 H           2.1143161291        -1.2666679892
       0.2942690181
 C           1.3291639008         0.7470858871
      -0.2342031883
 H           2.1143203820         1.2666386908
       0.2942397763
 H           0.9873290303         1.2552553298
      -1.1232168323
 H           0.9872734874        -1.2552917702
      -1.1231853006
 H           0.4259279322        -0.0000014755
       1.6583672292
```

substituents/22.xyz

```
  4
```

-9.25914020
H -2.9285804399 -0.0073273139
0.0010693632
C -1.8803181044 0.0017464235
0.0000667440
C -0.6818462772 -0.0015672757
-0.0003289103
CL 0.9512840271 0.0001476167
0.0000584173

substituents/35.xyz

8
-15.18256169
H 3.3421855711 -0.0052757246
0.0000983520
C 2.2903965611 -0.0077019424
0.0000196120
C 1.0889325211 -0.0325588299
-0.0000519279
B -0.4474709989 -0.0085752967
0.0000118221
O -1.1559404764 1.1570348648
-0.0000029873
H -0.6459639147 1.9642195138
0.0000898731
O -1.1180822613 -1.1767738753
0.0000074816
H -2.0701285111 -1.0738525933
-0.0000012584

substituents/28.xyz

```
  7
        -15.49551791
 H           3.2297494406         0.0485787833
       0.0000076148
 C           2.1795187406         0.0174982918
       0.0000021335
 C           0.9802633507        -0.0035678100
      -0.0000033881
 C          -0.4590228892        -0.0938666522
      -0.0000020601
 O          -1.0762469177        -1.1247919431
       0.0000010472
 O          -1.0290156510         1.1167977370
      -0.0000002185
 H          -1.9953817809         1.0309091056
       0.0000187301
```

substituents/16.xyz

```
  5
        -8.37905260
 H          -3.4831677880         0.0245924408
      -0.0000113655
 C          -2.4330397980         0.0163870005
      -0.0000030172
 C          -1.2320761480        -0.0408075299
       0.0000071109
 SE          0.5926576620         0.0215924495
      -0.0000004323
```

```
 H           0.7303735015        -1.4251528505
      -0.0000035495

substituents/20.xyz

  8
        -12.43931741
 H           2.8158028357        -0.5435640262
      -0.0000872596
 C           1.8099776364        -0.2575624036
       0.0000182292
 C           0.6823012274         0.1453866093
      -0.0000114424
 O          -0.5475781615         0.5726823624
      -0.0000039141
 C          -1.5431956840        -0.4336982151
      -0.0000009411
 H          -2.4994226627         0.0871066874
       0.0004959370
 H          -1.4674011954        -1.0643590081
      -0.8913242691
 H          -1.4668141159        -1.0648384424
       0.8909080609

substituents/33.xyz

  8
        -10.48953798
 H           2.8600880299         0.4637151188
      -0.0000039257
 C           1.8468476099         0.1920736990
```

```
      -0.0000011035
 C           0.6856110898       -0.1142401908
       0.0000022591
 C          -0.6737846002       -0.4923038906
      -0.0000002478
 C          -1.6744531601        0.3803746496
      -0.0000002463
 H          -1.4960361599        1.4429183095
       0.0000028027
 H          -2.7021944501        0.0598319097
      -0.0000046340
 H          -0.8571919804       -1.5601513706
      -0.0000021267

substituents/14.xyz

  8
        -20.64957099
 H           3.6129245098       -0.0606590329
      -0.0010812827
 C           2.5600908598       -0.0219413115
       0.0106161330
 C           1.3635869498        0.0203600698
       0.0189622983
 S          -0.3826131102        0.1040124027
       0.0444508097
 O          -0.7887911385        1.2375337073
      -0.7057139150
 O          -0.8251894922       -0.0877816473
       1.3888393333
 O          -0.7317508298       -1.2309538284
```

```
      -0.7829280818
 H          -0.9642708011        -1.9400015137
      -0.1810565895

substituents/6.xyz

  7
        -21.05114240
 H          -3.4433141610        -0.0000146950
      -0.0000064763
 C          -2.3926640210         0.0000161373
      -0.0000171456
 C          -1.1967022110        -0.0000133266
      -0.0000751896
 C           0.2610446990         0.0000005310
      -0.0000147207
 F           0.7622867608        -1.2439449461
      -0.0256177220
 F           0.7623566765         0.6441772322
      -1.0644354379
 F           0.7622326298         0.5997663808
       1.0901211853

substituents/31.xyz

  9
        -14.57453040
 H           3.2051766398         0.1480463397
       0.0000010179
 C           2.1569579998         0.0726521500
       0.0000248988
```

```
 C           0.9582990297         0.0014310004
      -0.0000347702
 C          -0.4791280003        -0.1181751291
      -0.0000165589
 O          -1.0443273407        -1.1828540289
       0.0000107520
 C          -1.1773614099         1.2176418611
       0.0000074011
 H          -0.8780955404         1.7845302607
      -0.8799265394
 H          -2.2548069699         1.0747705115
      -0.0002840979
 H          -0.8785515589         1.7842464114
       0.8802657106

substituents/12.xyz

  34
        -36.41411286
 H           1.2343870312        -1.0249469505
       3.8799548136
 C           0.9032223285        -0.7730581873
       2.9129496819
 C           0.5213907597        -0.4796465279
       1.8109289616
 SI          -0.0535785679        -0.0585332946
       0.0909026516
 C          -1.8639084297        -0.6917867634
      -0.0251877949
 C          -2.7321063051        -0.0866216817
       1.0740232746
```

```
H          -2.8078757766          0.9919929263
      0.9558726687
H          -3.7393124337         -0.5002785891
      1.0396332651
H          -2.3077843383         -0.2927278028
      2.0534832999
C          -2.4888687637         -0.4259333942
     -1.3923002374
H          -3.4903233233         -0.8526223927
     -1.4454405030
H          -2.5724590368          0.6438464047
     -1.5725629713
H          -1.8915526036         -0.8648937699
     -2.1886825763
H          -1.8510451669         -1.7746627558
      0.1323381948
C           1.0963751872         -1.0062254099
     -1.1203485285
H           0.8751119642         -0.7000576191
     -2.1481174011
C           2.5650498884         -0.6914206153
     -0.8476974236
H           2.8274727424         -0.9678238336
      0.1709499952
H           3.2094406764         -1.2451318070
     -1.5300261454
H           2.7705720723          0.3681876443
     -0.9753387576
C           0.8717977640         -2.5136322905
     -1.0268449404
H           1.5458442768         -3.0432063120
```

-1.6994561066
H -0.1484948573 -2.7752896415
-1.2950323830
H 1.0593879874 -2.8616277604
-0.0134503952
C 0.0238696198 1.8517517255
-0.1346680364
H -0.9400745938 2.2631265631
0.1828929107
C 0.2389592501 2.2626936377
-1.5907554836
H -0.5261945555 1.8406348609
-2.2381457651
H 0.2044424952 3.3476861823
-1.6881167097
H 1.2100894843 1.9260035061
-1.9463204814
C 1.0941092017 2.4875098935
0.7493506391
H 2.0832673951 2.1246094509
0.4814482146
H 1.0881448653 3.5712581332
0.6366480811
H 0.9203697851 2.2478922836
1.7950749416

substituents/37.xyz

14
-21.19676391
H 3.6323009283 0.8225256101

```
      -0.0001853997
 C          2.6452446493          0.4627849676
      -0.0001581401
 C          1.5006107402          0.1014052446
      -0.0000823905
 C          0.2026110719         -0.5416800588
       0.0000676089
 O          0.1071235551         -1.7551069991
       0.0001932986
 N         -0.8621224703          0.2947403484
      -0.0000037211
 C         -0.7701612440          1.7298381486
       0.0002114992
 H         -1.2619863648          2.1394849376
      -0.8870555108
 H         -1.2629026153          2.1392037971
       0.8871116092
 H          0.2735832752          2.0365906914
       0.0008076696
 C         -2.1942466688         -0.2560356851
      -0.0002662317
 H         -2.7400872894          0.0682994537
      -0.8897054717
 H         -2.1135353460         -1.3416391849
       0.0000553481
 H         -2.7406368299          0.0687705733
       0.8886679683

substituents/25.xyz

  10
```

```
         -18.66420596
 H            3.5585612074       -0.3745728987
       0.0005347777
 C            2.5545534973       -0.0796357190
       0.0003782280
 C            1.4223086971        0.3059076006
       0.0000034285
 O            0.1850657070        0.7373022102
      -0.0005138110
 C           -0.8409239627       -0.1584123102
      -0.0001930026
 O           -0.6852111723       -1.3441317801
      -0.0001070944
 C           -2.1486324629        0.5792160294
       0.0003505283
 H           -2.2051692330        1.2226190507
      -0.8750842407
 H           -2.9673824327       -0.1333977109
      -0.0086660029
 H           -2.2122842033        1.2070540880
       0.8866463593

substituents/18.xyz

  6
         -15.65509152
 H            3.1606696861        0.0000711551
      -0.0000291078
 C            2.1088551761        0.0000057538
      -0.0000272085
 C            0.9104108961        0.0000431023
```

```
       0.0000461308
 N          -0.4824129539          0.0000027306
       0.0000099599
 O          -1.0216510726         -1.0810877800
      -0.0000105447
 O          -1.0217399452          1.0810442300
      -0.0000105463

substituents/10.xyz

  14
        -20.09784636
 H           4.2294399491         -0.0001067008
      -0.0000880811
 C           3.1803571391         -0.0000498909
      -0.0000438910
 C           1.9798978291          0.0001039490
       0.0000000492
 C           0.5636826591          0.0000184889
       0.0000580093
 C          -0.1374896510          1.2055972088
       0.0000201701
 C          -1.5191760310          1.1999820087
      -0.0000042798
 C          -2.2123666609         -0.0000279314
      -0.0000370304
 C          -1.5191449408         -1.2000026713
      -0.0000157511
 C          -0.1374257208         -1.2056015512
       0.0000366187
 H           0.4093166693         -2.1374733211
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       0.0000090981
 H          -2.0594677607        -2.1356266014
      -0.0000598616
 H          -3.2924622809        -0.0000874515
      -0.0000097203
 H          -2.0595687711         2.1355585086
      -0.0001001392
 H           0.4092168889         2.1375018689
       0.0000831205

substituents/7.xyz

  10
        -32.65018188
 H          -3.3720181991        -1.8562166511
       0.0000213308
 C          -2.5626410793        -1.1863165009
      -0.0000216667
 C          -1.6411939095        -0.4238551706
       0.0000017748
 C          -0.5174997398         0.4985204197
       0.0000119845
 F          -0.5305981713         1.3104569391
      -1.0844413734
 F          -0.5305655388         1.3104436203
       1.0844410766
 C           0.8270605304        -0.2910904299
      -0.0000156493
 F           1.8815215302         0.5157317104
      -0.0000717084
 F           0.9102668794        -1.0757213204
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      -1.0761312918
 F          0.9102705619       -1.0756063394
       1.0762170582

substituents/23.xyz

  4
         -8.78478412
 H          3.4602830106       -0.0000035976
      -0.0000005932
 C          2.4115645606       -0.0000003365
      -0.0000000846
 C          1.2131638906        0.0000012388
       0.0000002527
 BR        -0.5885091194       -0.0000000902
      -0.0000000178

substituents/0.xyz

  4
         -5.20676978
 H          -1.6462174753        0.0029060705
      -0.0024870706
 C          -0.5970476641       -0.0001492566
       0.0004967450
 C          0.5970461169        -0.0004461346
      -0.0004071699
 H          1.6462359133         0.0041891212
       0.0014196178

substituents/29.xyz
```

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 10
       -18.65637432
H           3.5899382382          0.6890728576
     -0.0000944302
C           2.5738081081          0.4216927580
     -0.0000339004
C           1.4088080180          0.1364741584
      0.0000098294
C           0.0284788379         -0.2889242011
      0.0000073191
O          -0.3277290626         -1.4378375009
      0.0000094072
O          -0.7941071417          0.7665056193
      0.0000650511
C          -2.1811747918          0.4666604798
     -0.0000518790
H          -2.4449281018         -0.1150390016
      0.8860693901
H          -2.4458700523         -0.1097265986
     -0.8893628399
H          -2.6980140015          1.4227589500
      0.0030237928
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substituents/3.xyz

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 13
       -14.71220868
H           3.1590960443          0.0000289138
      0.3522172648
C           2.1326643741          0.0000069239
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       0.1357909951
 C           0.9644329504       -0.0000179597
      -0.1224746994
 C          -0.4603665356       -0.0000001537
      -0.4086655435
 C          -1.1072667579       -1.2621893703
       0.1674917193
 H          -0.9877773823       -1.2865312552
       1.2487554995
 H          -0.6437364819       -2.1536272369
      -0.2495901261
 H          -2.1698576633       -1.2794732541
      -0.0660582941
 C          -1.1072636179        1.2621952759
       0.1674891071
 H          -0.6432660877        2.1536299932
      -0.2490805691
 H          -2.1697193482        1.2798272082
      -0.0666512740
 H          -0.9883787647        1.2861999356
       1.2488266085
 H          -0.5876621930        0.0000086621
      -1.4990172748

substituents/21.xyz

  4
          -9.42778762
 H          -2.4158185836       -0.0006666198
      -0.0024306421
 C          -1.3694361612        0.0016602478
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       0.0002259975
 C          -0.1769312800        -0.0030501455
       0.0001238736
 F           1.1057943241         0.0009140742
      -0.0000922424

substituents/34.xyz

  5
          -9.69495525
 H           2.8583667474        -0.0000003467
       0.0000077147
 C           1.8106703674        -0.0000000193
       0.0000006603
 C           0.6084021574         0.0000003430
      -0.0000016799
 N          -0.6866433926        -0.0000004670
      -0.0000009753
 C          -1.8581983126         0.0000002500
       0.0000015095

substituents/27.xyz

  5
          -9.72662769
 H           2.9368301679        -0.0056640725
      -0.0006256258
 C           1.8872735038         0.0013908459
       0.0001357849
 C           0.6832303515        -0.0021134884
      -0.0000112129
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 C          -0.6823493547          0.0020971439
      -0.0001971480
 N          -1.8304564839         -0.0007710823
       0.0001072543

substituents/8.xyz

  13
        -44.26145142
 H          -0.0011947972         -3.9126555129
       0.6604148955
 C          -0.0008782659         -2.9072828518
       0.3560365091
 C          -0.0003536744         -1.7613122606
       0.0142480733
 C          -0.0000234925         -0.3719059891
      -0.4101373317
 F           0.0001078166         -0.2618721741
      -1.7789646213
 C           1.2837781090          0.3318447070
       0.1081361998
 F           1.3535535700          0.2805394821
       1.4392156296
 F           1.3420003008          1.6092019782
      -0.2517356856
 F           2.3690434277         -0.2723614330
      -0.3712169732
 C          -1.2836160410          0.3322746111
       0.1080073219
 F          -2.3690804123         -0.2724003655
      -0.3702924295
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 F          -1.3527531700          0.2819643164
       1.4392719517
 F          -1.3421169092          1.6092990425
      -0.2527670835

substituents/15.xyz

  20
        -23.19885137
 H           4.2348399201          0.0006003206
       0.4377226916
 C           3.2141966203          0.0001519403
       0.1956463209
 C           2.0531659605         -0.0002323901
      -0.0941966997
 C           0.6381114706         -0.0002605706
      -0.4157395906
 H           0.5331698413         -0.0003021199
      -1.5084936706
 C          -0.0384909203          1.2561950588
       0.1467631198
 C          -1.5269768901          1.2533807183
      -0.1873018511
 C          -2.1985260898          0.0002340776
       0.3669805277
 C          -1.5273113489         -1.2531180517
      -0.1872761527
 H          -2.0002730287         -2.1449161122
       0.2297483465
 C          -0.0388222791         -1.2564393012
       0.1468608582
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 H           0.4387284515       -2.1476144807
      -0.2667381820
 H           0.0949664703       -1.2781620818
       1.2311518083
 H          -1.6564972183       -1.2836559411
      -1.2722871428
 H          -2.1208079105        0.0002378070
       1.4569085978
 H          -3.2593939997        0.0003957773
       0.1073359071
 H          -1.6561597394        1.2840134089
      -1.2723348711
 H          -1.9996164707        2.1453124778
       0.2297840792
 H           0.0953594891        1.2779806082
       1.2309986099
 H           0.4393620496        2.1471651993
      -0.2669844794

substituents/32.xyz

  6
         -9.42852736
 H          -2.9323082405       -0.0000286131
      -0.0000462598
 C          -1.8839984605        0.0000049917
      -0.0000176461
 C          -0.6801432705        0.0000354827
       0.0000292839
 C           0.6801473595       -0.0000781745
       0.0000070533
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 C           1.8839946695         0.0000361741
      -0.0000132757
 H           2.9323046895         0.0000467988
      -0.0000182753

substituents/1.xyz

  7
         -8.38291033
 H           2.4001599818        -0.0000046133
      -0.0000146153
 C           1.3516163818        -0.0000045784
       0.0000056246
 C           0.1554719918         0.0000098492
      -0.0000076387
 C          -1.2900472882        -0.0000028881
       0.0000019940
 H          -1.6622029483        -0.6180070614
      -0.8168225064
 H          -1.6622148477         1.0163890754
      -0.1267811615
 H          -1.6621897284        -0.3984057958
       0.9436185232

substituents/13.xyz

  37
        -52.57021751
 H          -0.0007628038         0.0033533940
      -4.7425809494
 C          -0.0006862231         0.0026316231
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-3.6900486294
C -0.0007788822 0.0011324321
-2.4878127294
SI -0.0004013711 0.0003869006
-0.6286072694
C -1.7360529083 0.4597076915
-0.0328895082
C -2.3565981728 1.6101121902
-0.5110147669
C -3.6189327093 1.9712007818
-0.0777320659
C -4.2853756314 1.1829058095
0.8460863237
C -3.6826597973 0.0344277670
1.3303523324
C -2.4192338920 -0.3214268343
0.8929367315
H -1.9549788609 -1.2206082561
1.2742074205
H -4.1988878155 -0.5845096832
2.0505835822
H -5.2718367107 1.4629546197
1.1867887345
H -4.0857096899 2.8682759930
-0.4592108449
H -1.8393194640 2.2263220506
-1.2329579666
C 1.2659299189 1.2732923289
-0.0332611190
C 2.5722553769 1.2348571767
-0.5119650897

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C          3.5169981535        2.1465104569
     -0.0784435294
C          3.1686356678        3.1174272022
      0.8461980416
C          1.8728770268        3.1704016166
      1.3309498423
C          0.9321147109        2.2551737073
      0.8932962020
H         -0.0785481891        2.3032069723
      1.2749777926
H          1.5958543966        3.9266344772
      2.0518332131
H          3.9051032465        3.8308425783
      1.1871750819
H          4.5270907628        2.1016995517
     -0.4603525799
H          2.8464086970        0.4790357156
     -1.2345082005
C          0.4697195272       -1.7326465401
     -0.0336657912
C          1.4884975604       -1.9340506846
      0.8913129081
C          1.8119367008       -3.2062224763
      1.3285390769
C          1.1178691032       -4.3022044433
      0.8449392163
C          0.1012835138       -4.1188870883
     -0.0780620230
C         -0.2170689269       -2.8450412655
     -0.5111697318
H         -1.0099305570       -2.7049377133
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-1.2324408413
H -0.4428042853 -4.9714974735
-0.4590686435
H 1.3684871145 -5.2965973103
1.1855036653
H 2.6066234904 -3.3440543982
2.0481092964
H 2.0356943198 -1.0825771387
1.2720882486

substituents/38.xyz

10
-24.66653758
H 3.9431123818 0.5278973651
-0.0483480857
C 2.9655925713 0.1555898963
-0.0317129876
C 1.8708571307 -0.3191710026
0.0274129700
O 0.6784407500 -0.8500622812
0.0556778273
P -0.6334257888 0.1065256004
0.0867867821
O -0.5750740373 1.2648589859
0.9605613679
O -1.7378476602 -0.9686761098
0.4010840567
H -1.7387351111 -1.6986571767
-0.2188258669
O -0.8564614283 0.4558642984

-1.4649060261
H -0.8326494870 1.4023871391
-1.5932979314

substituents/4.xyz

16
-17.87990093
H -3.3422664714 -0.0000148814
-0.0000936755
C -2.2931233814 -0.0001322003
0.0000276841
C -1.0966730914 -0.0001766303
0.0000232527
C 0.3606152486 -0.0000067603
0.0000110891
C 0.8567039266 -0.4631579117
-1.3747877710
H 1.9446819366 -0.4703689603
-1.3970643783
H 0.4966383855 0.2049561254
-2.1543782392
H 0.4971036264 -1.4670358693
-1.5909149672
C 0.8568546803 -0.9589064021
1.0885432505
H 1.9448373803 -0.9744260474
1.1058826773
H 0.4969463800 -1.9681815954
0.8998021924
H 0.4972461817 -0.6441539046

2.0659884339
C 0.8564009690 1.4223074322
0.2862012732
H 0.4965470178 2.1113356027
-0.4750705615
H 1.9443724390 1.4454439748
0.2909745853
H 0.4963717604 1.7633091995
1.2546501525

substituents/26.xyz

11
-36.48585975
H -3.7838583828 -1.7597218344
-0.5459753518
C -3.0219174046 -1.1466900456
-0.1702619774
C -2.1905513099 -0.4406474514
0.3186547637
O -1.2665445970 0.3220459275
0.8478583187
S -0.0934438061 0.8936364727
-0.0835529888
O -0.5242642541 1.0247399075
-1.4261858728
O 0.5208698636 1.9576198872
0.6114177100
C 1.0737530306 -0.5840720054
-0.0036537551
F 2.1927118672 -0.3206344883

-0.6588634741
F 1.3623256054 -0.8604047858
1.2597734556
F 0.4894049649 -1.6436233847
-0.5503207618

substituents/30.xyz

6
-8.64167056
H 2.3835912399 -0.0000012465
0.0267016045
C 1.3380214800 -0.0000076291
-0.0089984770
C 0.1394308400 0.0000144382
-0.0056971889
N -1.2043042001 -0.0000052444
0.0563087491
H -1.6270324714 0.8402476422
-0.3170454271
H -1.6270341877 -0.8402546578
-0.3170478960

substituents/19.xyz

5
-9.27869674
H 2.3820266673 -0.0048672507
0.0000237475
C 1.3368987573 0.0111043793
-0.0000047119

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 C           0.1410451973         0.0002738293
      0.0000036186
 O          -1.1620466027        -0.0600683108
     -0.0000006811
 H          -1.5481507127         0.8227988592
      0.0000000940

substituents/11.xyz

  16
        -17.43471652
 H          -3.7575667927        -0.0004975892
     -0.0007438871
 C          -2.7049594732        -0.0002489191
     -0.0004248493
 C          -1.5026989622        -0.0000302787
     -0.0002589697
 SI          0.3584946962         0.0000375926
      0.0000564632
 C           0.9573175485        -0.3594881380
     -1.7738506040
 H           0.5978645298        -1.3232508457
     -2.1220198636
 H           2.0421750758        -0.3723462924
     -1.8317938717
 H           0.5996349637         0.3937327269
     -2.4695375863
 C           0.9561023658         1.7164144835
      0.5758346399
 H           0.5993877419         1.9412323438
      1.5765694692
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 H           0.5946727710         2.4997048644
      -0.0837818783
 H           2.0409056204         1.7745210606
       0.5922819251
 C           0.9564003292        -1.3567338119
       1.1985046068
 H           0.5979145961        -2.3354959668
       0.8939265823
 H           2.0412198118        -1.4014084941
       1.2386170530
 H           0.5970328092        -1.1762065733
       2.2072345783

substituents/9.xyz

  16
        -55.88475453
 H          -0.0004720579         0.0016089332
      -4.0246163108
 C          -0.0002976208         0.0012211073
      -2.9744309708
 C          -0.0000847759         0.0003968487
      -1.7791899308
 C           0.0000004673         0.0000246979
      -0.3236881208
 C          -0.6876953243         1.2935545016
       0.1885661940
 F          -0.9915005719         1.2239005894
       1.4813682935
 F          -1.8170379698         1.5316388526
      -0.4745677092
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 F           0.0992481674         2.3535264094
      0.0165466830
 C           1.4642041190        -0.0513176915
      0.1881626927
 F           1.5560717245         0.2461717872
      1.4810542621
 F           2.2348784177         0.8079229767
     -0.4748558778
 F           1.9886910651        -1.2627381960
      0.0156116273
 C          -0.7764400399        -1.2424775801
      0.1880248407
 F          -0.5645130742        -1.4711090880
      1.4808175319
 F          -0.4177694411        -2.3393409544
     -0.4753285954
 F          -2.0878452817        -1.0909440203
      0.0157547673

substituents/36.xyz

  8
       -14.85852152
 H           3.2170061301        -0.0369747414
      0.0000700855
 C           2.1665203301        -0.0175187808
      0.0000288673
 C           0.9671380001        -0.0143719102
     -0.0000377906
 C          -0.4787594599         0.0869258305
     -0.0000349582
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 O          -1.0700486893          1.1413129608
       0.0000029431
 N          -1.0933471405         -1.1225134492
       0.0000677726
 H          -0.5756402409         -1.9828574694
      -0.0005116184
 H          -2.0993160205         -1.1537371086
      -0.0000240857

substituents/24.xyz

  4
         -8.51180167
 H           3.8226195663         -0.0000028253
      -0.0000030562
 C           2.7731899063          0.0000026031
       0.0000020563
 C           1.5758729763         -0.0000036467
      -0.0000027344
 I          -0.4419812737          0.0000001212
       0.0000000885
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