

Supporting Information:

Electron Spin-Lattice Relaxation in Triplet-State Oligoacenes: A First-Principles-Based Approach

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1 Derivation of the Redfield Master Equation

We assume that the total Hamiltonian can be divided into the system, environment and their interaction terms.

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{H}_I. \quad (1)$$

Then, the time evolution of the whole density matrix are governed by the Liouville-von Neumann equation,

$$\frac{d}{dt}\hat{\rho}(t) = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}(t)]. \quad (2)$$

By tracing out the degrees of freedom of the environment, we can obtain a master equation describing the reduced dynamics of the system. Here, assuming that the interaction between the system and the bath is weak and the bath dynamics is faster than the system dynamics, the master equation applying the Born-Markov approximation can be obtained.

$$\frac{d}{dt}\hat{\rho}_S(t) = -\frac{1}{\hbar^2} \int_0^\infty d\tau \text{Tr}_B \left[\hat{H}_I(t), \left[\hat{H}_I(t-\tau), \hat{\rho}_S(t) \otimes \hat{\rho}_B^{\text{eq}} \right] \right], \quad (3)$$

where the interaction picture is used. This equation is rather general and difficult to handle, so we assume a specific form of the system-bath interaction Hamiltonian as

$$\hat{H}_I = \sum_{\alpha} \hat{V}_{\alpha} \otimes \hat{Q}_{\alpha}, \quad (4)$$

where Hermite operator $\hat{V}_\alpha$ and $\hat{Q}_\alpha$ act only on system and environment variables, respectively. Substituting this into eq. (3) becomes

$$\begin{aligned} \frac{d}{dt}\hat{\rho}_S(t) = & -\frac{1}{\hbar^2} \sum_{\alpha,\beta} \int_0^\infty d\tau \left[\left\{ \hat{V}_\alpha(t)\hat{V}_\beta(t-\tau)\hat{\rho}_S(t) - \hat{V}_\beta(t-\tau)\hat{\rho}_S(t)\hat{V}_\alpha(t) \right\} C_{\alpha\beta}(t, t-\tau) \right. \\ & \left. + \left\{ \hat{\rho}_S(t)\hat{V}_\beta(t-\tau)\hat{V}_\alpha(t) - \hat{V}_\alpha(t)\hat{\rho}_S(t)\hat{V}_\beta(t-\tau) \right\} C_{\beta\alpha}(t-\tau, t) \right], \quad (5) \end{aligned}$$

here the bath correlation function is defined as

$$C_{\alpha\beta}(t, t') = \text{Tr}_B \left[\hat{Q}_\alpha(t)\hat{Q}_\beta(t')\hat{\rho}_B^{\text{eq}} \right]. \quad (6)$$

Because $\hat{\rho}_B^{\text{eq}}$ is a bath density matrix of the stationary state, i.e., $[\hat{H}_B, \hat{\rho}_B^{\text{eq}}] = 0$, the time evolution operator $e^{-\frac{i\hat{H}_B t}{\hbar}}$ commutes with $\hat{\rho}_B^{\text{eq}}$ and the following holds for the correlation function,

$$C_{\alpha\beta}(t, t') = C_{\alpha\beta}(t - t', 0) \quad (7)$$

$$C_{\alpha\beta}(t, t') = C_{\beta\alpha}^*(t', t). \quad (8)$$

From eq. (8), it is evident that the latter part of eq. (5) is the Hermitian conjugate of the former part.

Returning eq. (5) to the Schrödinger picture gives

$$\begin{aligned} \frac{d}{dt}\hat{\rho}_S(t) = & -\frac{i}{\hbar} [\hat{H}_S, \hat{\rho}_S(t)] \\ & - \frac{1}{\hbar^2} \sum_{\alpha,\beta} \int_0^\infty d\tau \left[\left\{ \hat{V}_\alpha e^{-\frac{i\hat{H}_S\tau}{\hbar}} \hat{V}_\beta e^{\frac{i\hat{H}_S\tau}{\hbar}} \hat{\rho}_S(t) - e^{-\frac{i\hat{H}_S\tau}{\hbar}} \hat{V}_\beta e^{\frac{i\hat{H}_S\tau}{\hbar}} \hat{\rho}_S(t) \hat{V}_\alpha \right\} C_{\alpha\beta}(\tau, 0) \right. \\ & \left. + \left\{ \hat{\rho}_S(t) e^{-\frac{i\hat{H}_S\tau}{\hbar}} \hat{V}_\beta e^{\frac{i\hat{H}_S\tau}{\hbar}} \hat{V}_\alpha - \hat{V}_\alpha \hat{\rho}_S(t) e^{-\frac{i\hat{H}_S\tau}{\hbar}} \hat{V}_\beta e^{\frac{i\hat{H}_S\tau}{\hbar}} \right\} C_{\beta\alpha}(-\tau, 0) \right]. \quad (9) \end{aligned}$$

Next, taking the eigenstates of $\hat{H}_S$ as the basis, this equation becomes

$$\begin{aligned} \frac{d}{dt}\rho_{ab}(t) = & -i\omega_{ab}\rho_{ab}(t) \\ & - \frac{1}{\hbar^2} \sum_{c,d} \sum_{\alpha,\beta} \int_0^\infty d\tau \left[\left\{ V_{ac}^\alpha V_{cd}^\beta \rho_{db}(t) e^{i\omega_{dc}\tau} - V_{ac}^\beta \rho_{cd}(t) V_{db}^\alpha e^{i\omega_{ca}\tau} \right\} C_{\alpha\beta}(\tau, 0) \right. \\ & \left. + \left\{ \rho_{ac}(t) V_{cd}^\beta V_{db}^\alpha e^{i\omega_{dc}\tau} - V_{ac}^\alpha \rho_{cd}(t) V_{db}^\beta e^{i\omega_{bd}\tau} \right\} C_{\beta\alpha}(-\tau, 0) \right]. \quad (10) \end{aligned}$$

Here, by setting $\Gamma_{\alpha\beta}(\omega) = \int_0^\infty d\tau e^{i\omega\tau} C_{\alpha\beta}(\tau, 0)$, it can be decomposed as

$$\Gamma_{\alpha\beta}(\omega) = G_{\alpha\beta}(\omega) + i\Lambda_{\alpha\beta}(\omega) \quad (11)$$

$$\begin{cases} G_{\alpha\beta}(\omega) = \frac{1}{2} (\Gamma_{\alpha\beta}(\omega) + \Gamma_{\beta\alpha}^*(\omega)) = \frac{1}{2} \int_{-\infty}^\infty d\tau e^{i\omega\tau} C_{\alpha\beta}(\tau, 0) \\ \Lambda_{\alpha\beta}(\omega) = \frac{1}{2i} (\Gamma_{\alpha\beta}(\omega) - \Gamma_{\beta\alpha}^*(\omega)) \end{cases} \quad (12)$$

where $G_{\alpha\beta}(\omega)$ is noise-power spectrum and $\Lambda_{\alpha\beta}(\omega)$ is the Lamb shift part of spectral density. $\Lambda_{\alpha\beta}(\omega)$ contributes to the coherence motion as an energy shift, but it is ignored here. Also, by neglecting the cross-correlation between the bath degrees of freedom, $G_\alpha(\omega)$ can be taken as a real function, and eq. (10) becomes as follows,

$$\begin{aligned} \frac{d}{dt}\rho_{ab}(t) = & -i\omega_{ab}\rho_{ab}(t) \\ & - \frac{1}{\hbar^2} \sum_{c,d} \sum_{\alpha} \{ V_{ac}^\alpha V_{cd}^\alpha G_\alpha(\omega_{dc}) \rho_{db}(t) - V_{ac}^\alpha V_{db}^\alpha G_\alpha(\omega_{ca}) \rho_{cd}(t) \\ & + V_{cd}^\alpha V_{db}^\alpha G_\alpha(\omega_{cd}) \rho_{ac}(t) - V_{ac}^\alpha V_{db}^\alpha G_\alpha(\omega_{db}) \rho_{cd}(t) \}. \quad (13) \end{aligned}$$

Consolidating the relaxation terms into the tensor $R_{ab,cd}$, the desired Redfield equation is

obtained.

$$\frac{d}{dt}\rho_{ab}(t) = -i\omega_{ab}\rho_{ab}(t) - \sum_{c,d} R_{ab,cd}\rho_{cd}(t) \quad (14)$$

$$R_{ab,cd} = \frac{1}{\hbar^2} \sum_{\alpha} \left\{ \delta_{bd} \sum_j V_{aj}^{\alpha} V_{jc}^{\alpha} G_{\alpha}(\omega_{cj}) - V_{ac}^{\alpha} V_{db}^{\alpha} G_{\alpha}(\omega_{ca}) \right. \\ \left. + \delta_{ac} \sum_j V_{dj}^{\alpha} V_{jb}^{\alpha} G_{\alpha}(\omega_{dj}) - V_{ac}^{\alpha} V_{db}^{\alpha} G_{\alpha}(\omega_{db}) \right\}. \quad (15)$$

2 SLR from the Fluctuation of g Tensor

We evaluated the contribution of fluctuations in the electron Zeeman splitting to the SLR rates. The calculation method followed the same Redfield theory described in the main text, where the spin-phonon couplings were obtained by computing the derivative of the g tensor along each normal mode. Normal modes were taken from the *p*-terphenyl host environment, and the g tensors were computed at the UPBE/def2-SVP level of theory with the use of GIAO and SOMF approach for SOC integrals implemented in ORCA program. In the DFT calculations, the host environment was incorporated using RESP charges. The derivative values of g_{ZZ} are shown in Figure S1. The resulting SLR rate constants at 300 K under magnetic field $\mathbf{B}/T = (1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$ were as follows: $k_{+0} = 6.00 \times 10^{-5} \text{ ms}^{-1}$, $k_{0-} = 6.12 \times 10^{-5} \text{ ms}^{-1}$, and $k_{+-} \approx 0 \text{ ms}^{-1}$. Although the rates roughly scale with the square of the magnetic field strength, it is significantly smaller than the SLR rates arising from D tensor fluctuations over the magnetic field range used in typical experiments. This indicates that the contribution of g tensor to the SLR is negligible for pentacene molecules. This is attributed to the small spin-orbit coupling, which leads to correspondingly small derivatives of the g tensor.

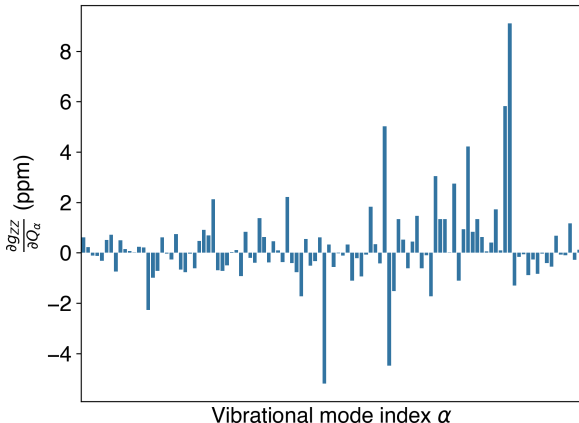


Figure S1: Derivative values of g_{ZZ} along the Z-direction of the ZFS principal axis.

3 Symmetry-Broken Unphysical Solutions of CASSCF

When performing CASSCF calculations with an active space truncated to valence π orbitals, there may exist the lower energy solution with reduced molecular orbital symmetry. This solution also break the symmetry of the spin density and cause significant changes significant changes in the orientation of the principal axes of the D tensor. Symmetry-broken occurs more frequently when the molecular structure has low symmetry becomes a problem when the structure is shifted for numerical differentiation of the D tensor.

Here, as a demonstration, the CASSCF(12e,12o) calculations of pentacene is taken as an example. At the equilibrium geometry of the T_1 state, the energy and D tensor obtained from CASSCF calculations using MolPro and PySCF are as follows.

$$E/E_h = -841.39690141, \quad \mathbf{D}/\text{cm}^{-1} = \begin{pmatrix} -0.0202 & 0 & 0 \\ 0 & -0.0089 & 0 \\ 0 & 0 & 0.0292 \end{pmatrix}.$$

Then, the CASSCF is performed for a geometry shifted along the normal mode Q_7 (b_{1g} , 231 cm^{-1}) by dimensionless length 0.05. Below is the output of the macro iterations of the SCF cycle.

ITER.	MIC	NCI	ENERGY	ENERGY CHANGE	GRAD	ORB GRAD
1	2	27	-841.39689625	-841.39689625	0.00315505	0.00315505
2	2	5	-841.39689950	-0.00000325	0.00075908	0.00075907
3	7	5	-841.39689975	-0.00000025	0.00021690	0.00021687
4	3	5	-841.39725897	-0.00035922	0.01044648	0.01042241
5	3	5	-841.39806721	-0.00080824	0.01614479	0.01612579
6	2	5	-841.39871029	-0.00064308	0.01393899	0.01391958
7	2	5	-841.39899988	-0.00028959	0.00917762	0.00906707
8	3	5	-841.39913559	-0.00013571	0.00368693	0.00367817
9	2	5	-841.39914986	-0.00001427	0.00086029	0.00085678
10	2	6	-841.39915226	-0.00000240	0.00040808	0.00040745
11	2	6	-841.39915259	-0.00000034	0.00017154	0.00017136
12	2	6	-841.39915263	-0.00000004	0.00006390	0.00006388
13	2	6	-841.39915264	-0.00000000	0.00002853	0.00002852

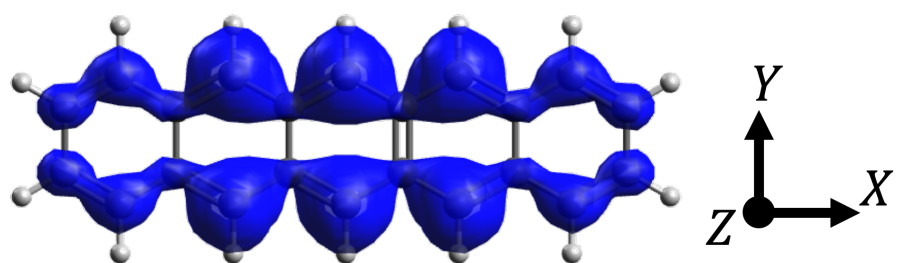
The energy converged at the iteration 13 shows a much lower value than that of the equilibrium geometry. On the other hand, there is a stationary point around the iteration

3, and its energy is slightly higher than that of the equilibrium geometry, which is the originally expected solution. The D tensor was calculated for the converged solution and the terminated solution at the iteration 3, and the results are as follows.

$$\begin{aligned} \mathbf{D}_{\text{Iter.3}}/\text{cm}^{-1} &= \begin{pmatrix} -0.0202 & 0 & 0 \\ 0 & -0.0089 & 0 \\ 0 & 0 & 0.0292 \end{pmatrix}, \\ \mathbf{D}_{\text{Iter.13}}/\text{cm}^{-1} &= \begin{pmatrix} -0.0215 & 0.0026 & 0 \\ 0.0026 & -0.0077 & 0 \\ 0 & 0 & 0.0293 \end{pmatrix}. \end{aligned}$$

$\mathbf{D}_{\text{Iter.3}}$ showed almost no change compared to the $\mathbf{D}$ at the equilibrium geometry. Surprisingly, however, $\mathbf{D}_{\text{Iter.13}}$, corresponding to the lower-energy solution, exhibited a significant in-plane rotation in the XY plane. From the Figure S2, it was in fact confirmed that the symmetry of the spin density is broken in the converged structure. Thus, the derivative of D tensor at the iteration 13 become $\frac{\partial D_{XY}}{\partial Q_7} = 0.052 \text{ cm}^{-1}$, and when converted to the SLR rate constant at 300 K, it results in $k_{XY} = 2170 \text{ ms}^{-1}$, which is significantly faster than the experimental value of several tens of ms^{-1} .

Iter. 3



Iter. 13

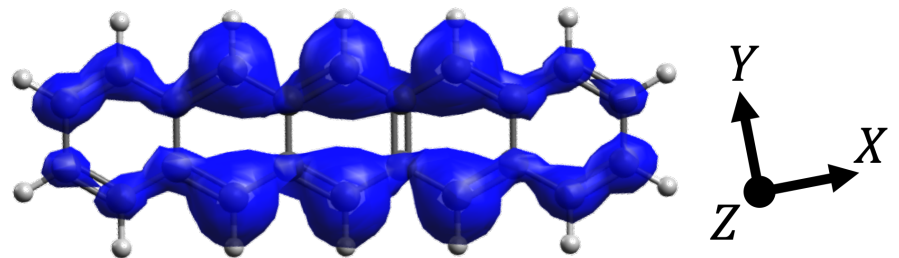


Figure S2: Plot of the spin densities (isovalue=0.001). The coordinate axes represent the principal axes of D tensor.

4 Selection Rules for SLR Anisotropy

4.1 In the zero field limit

Using the principal axes coordinate system of the ZFS, spin-phonon coupling can be expressed as follows.

$$V_{ab}^\alpha = \sum_{i,j \in \{X,Y,Z\}} \frac{\partial D_{ij}}{\partial Q_\alpha} \langle a | \hat{S}_i \hat{S}_j | b \rangle. \quad (16)$$

The matrix elements of the spin operator are

$$\langle i | \hat{S}_i \hat{S}_j | i \rangle = 1, \quad (i \neq j) \quad (17)$$

$$\langle X | \hat{S}_Z \hat{S}_X | Z \rangle = \langle Z | \hat{S}_X \hat{S}_Z | X \rangle = 1,$$

$$\langle Y | \hat{S}_X \hat{S}_Y | X \rangle = \langle Z | \hat{S}_Y \hat{S}_Z | Y \rangle = i,$$

$$\langle X | \hat{S}_Y \hat{S}_X | Y \rangle = \langle Y | \hat{S}_Z \hat{S}_Y | Z \rangle = -i,$$

$$(\text{The others}) = 0.$$

Since eq.(17) does not contribute to the relaxation, only one term contributes to each of the six possible transitions. When molecular symmetry is present, additional selection rules for the derivative values of the D tensor can be derived. Here, we consider the case where the molecular point group follows D_{2h} , which applies to some oligoacenes, including pentacene. Because the symmetry of the principal axes follows the molecular point group, the components of the D tensor obey the irreducible representations of quadratic forms (Table S1). For $\frac{\partial D_{ij}}{\partial Q_\alpha}$ to be nonzero, the irreducible representation of the component of the D tensor must match that of the normal mode. Therefore, when combined with the selection rules of the spin operator, only normal modes with b_{1g} , b_{2g} , and b_{3g} contribute to k_{XY} , k_{XZ} , and k_{YZ} , respectively.

Table S1: Irreducible representations followed by quadratic forms in the D_{2h} point group.

Irrep.	a_g	b_{1g}	b_{2g}	b_{3g}	$\dots$
Quadratic	x^2, y^2, z^2	xy	xz	yz	

4.2 In the high field limit

Under a high magnetic field, spin sublevels are well-characterized by their magnetic quantum number, and it is more useful to expand spin-phonon coupling in the spherical tensor basis.

$$V_{ab}^\alpha = \sum_{k=-2}^2 (-1)^k \frac{\partial D_{-k}^{(2)}}{\partial Q_\alpha} \langle a | \left[\hat{S} \otimes \hat{S} \right]_k^{(2)} | b \rangle, \quad (18)$$

where the summation is taken only over five components from the second-rank spherical tensor because the D tensor is traceless and symmetric. By considering the Wigner-Eckart theorem and the conditions under which the Clebsch-Gordan coefficients become nonzero, the selection rules for the matrix elements of the spin operator are determined to be

$$\begin{aligned} \langle a | \left[\hat{S} \otimes \hat{S} \right]_k^{(2)} | b \rangle &\neq 0 \quad (a = k + b) \\ &= 0. \quad (\text{The others}) \end{aligned}$$

From this, only one term contributes to each of the six transitions. For the components of the D tensor, further analysis can be achieved by transforming into the Cartesian basis.

$$\begin{aligned} D_2^{(2)} &= \frac{1}{2} (D_{XX} - D_{YY}) + iD_{XY}, \\ D_1^{(2)} &= D_{XZ} + iD_{YZ}, \\ D_0^{(2)} &= \frac{1}{\sqrt{6}} (2D_{ZZ} - D_{XX} - D_{YY}), \\ D_{-1}^{(2)} &= D_{XZ} - iD_{YZ}, \\ D_{-2}^{(2)} &= \frac{1}{2} (D_{XX} - D_{YY}) - iD_{XY}, \end{aligned}$$

where Z is aligned with the direction of the quantization axis. If the magnetic field is applied along the molecular symmetry axis, it is possible to determine which components contribute by considering irreducible representations, similar to the case of zero-field limit.

5 Effect of RESP Point Charges on SLR Rates

Table S2: SLR rate constants of pentacene in zero magnetic field and 300K. The same set of normal modes was used for each host-guest system. In the CASSCF calculations of the D tensors, the table shows the results for the following three cases: (1) only the structure of pentacene was used; (2) all surrounding host molecules were replaced with RESP charges; and (3) six *p*-terphenyl molecules or six set of benzoic acid dimers expected to overlap with the π orbitals of pentacene were treated with the STO-3G basis set, while the remaining host molecules were replaced with RESP charges.

	k_{XZ}		k_{YZ}		k_{XY}	
	$Q_\alpha(\omega_\alpha/\text{cm}^{-1})$	$k_{XZ}^{(\alpha)}/\text{ms}^{-1}$	$Q_\alpha(\omega_\alpha/\text{cm}^{-1})$	$k_{YZ}^{(\alpha)}/\text{ms}^{-1}$	$Q_\alpha(\omega_\alpha/\text{cm}^{-1})$	$k_{XY}^{(\alpha)}/\text{ms}^{-1}$
<i>p</i>-terphenyl No RESP	Total	0.67	Total	4.81	Total	0.22
	$Q_7(101)$	0.18	$Q_7(101)$	2.51	$Q_{26}(497)$	0.06
	$Q_4(80)$	0.17	$Q_{11}(174)$	0.95	$Q_{89}(1507)$	0.04
<i>p</i>-terphenyl Full RESP	Total	0.64	Total	4.86	Total	0.19
	$Q_5(81)$	0.17	$Q_7(101)$	2.56	$Q_{26}(497)$	0.07
	$Q_4(80)$	0.17	$Q_{11}(174)$	0.95	$Q_{22}(442)$	0.03
<i>p</i>-terphenyl Mixed STO-3G/RESP	Total	0.64	Total	4.81	Total	0.18
	$Q_5(81)$	0.20	$Q_7(101)$	2.52	$Q_{26}(497)$	0.07
	$Q_4(80)$	0.20	$Q_{11}(174)$	0.97	$Q_{22}(442)$	0.03
Benzoic acid No RESP	Total	0.73	Total	5.11	Total	0.19
	$Q_4(77)$	0.67	$Q_7(100)$	3.49	$Q_{22}(440)$	0.04
	$Q_{16}(305)$	0.02	$Q_{11}(173)$	1.09	$Q_{94}(1582)$	0.03
Benzoic acid Full RESP	Total	0.96	Total	4.89	Total	0.17
	$Q_4(77)$	0.78	$Q_7(100)$	3.42	$Q_{26}(496)$	0.06
	$Q_7(100)$	0.07	$Q_{11}(173)$	1.05	$Q_{22}(440)$	0.02
Benzoic acid Mixed STO-3G/RESP	Total	0.89	Total	4.91	Total	0.18
	$Q_4(77)$	0.73	$Q_7(100)$	3.42	$Q_{26}(496)$	0.06
	$Q_7(100)$	0.06	$Q_{11}(173)$	1.06	$Q_{22}(440)$	0.02

6 Raman Relaxation

We performed calculations of the Raman relaxation component of the SLR rate. Raman relaxation contains two types of contributions: (1) the term arising from the first-order term in the Herzberg–Teller expansion of the spin-phonon coupling combined with the fourth-order term in the perturbation expansion, and (2) the term arising from the second-order term in the Herzberg–Teller expansion of the spin-phonon coupling combined with the second-order term in the perturbation expansion. For case (1), the transition rate constant from state a to state b can be expressed as follows.^{S1}

$$k_{ab} = \frac{\pi}{2\hbar} \sum_{\alpha \leq \beta} (A_{\alpha\beta} W_{ab}^{--} + A_{\alpha\beta} W_{ab}^{++} + B_{\alpha\beta} W_{ab}^{+-} + B_{\alpha\beta} W_{ab}^{-+}), \quad (19)$$

$$\begin{aligned} W_{ab}^{--} &= \left| \sum_c \left[\frac{V_{ac}^\alpha V_{cb}^\beta}{E_c - E_b - \hbar\omega_\beta} + \frac{V_{ac}^\beta V_{cb}^\alpha}{E_c - E_b - \hbar\omega_\alpha} \right] \right|^2 \bar{n}_\alpha \bar{n}_\beta \delta(\omega_{ba} - \omega_\alpha - \omega_\beta), \\ W_{ab}^{++} &= \left| \sum_c \left[\frac{V_{ac}^\alpha V_{cb}^\beta}{E_c - E_b + \hbar\omega_\beta} + \frac{V_{ac}^\beta V_{cb}^\alpha}{E_c - E_b + \hbar\omega_\alpha} \right] \right|^2 (\bar{n}_\alpha + 1)(\bar{n}_\beta + 1) \delta(\omega_{ba} + \omega_\alpha + \omega_\beta), \\ W_{ab}^{+-} &= \left| \sum_c \left[\frac{V_{ac}^\alpha V_{cb}^\beta}{E_c - E_b + \hbar\omega_\beta} + \frac{V_{ac}^\beta V_{cb}^\alpha}{E_c - E_b - \hbar\omega_\alpha} \right] \right|^2 \bar{n}_\alpha (\bar{n}_\beta + 1) \delta(\omega_{ba} - \omega_\alpha + \omega_\beta), \\ W_{ab}^{-+} &= \left| \sum_c \left[\frac{V_{ac}^\alpha V_{cb}^\beta}{E_c - E_b - \hbar\omega_\beta} + \frac{V_{ac}^\beta V_{cb}^\alpha}{E_c - E_b + \hbar\omega_\alpha} \right] \right|^2 (\bar{n}_\alpha + 1) \bar{n}_\beta \delta(\omega_{ba} + \omega_\alpha - \omega_\beta), \end{aligned}$$

where $A_{\alpha\beta} = 1 - \frac{3}{4}\delta_{\alpha\beta}$ and $B_{\alpha\beta} = 1 - \frac{1}{2}\delta_{\alpha\beta}$. Note that the sign convention of ω appearing through the Fourier transform in the spectral density is opposite to that used in the main text. Using the same Lorentzian spectral density as employed in the main text,

$$\delta(\omega_{ba} - \omega_\alpha - \omega_\beta) \approx \frac{1}{\pi} \frac{\Delta_{\alpha\beta}}{\Delta_{\alpha\beta}^2 + \hbar^2(\omega_{ba} - \omega_\alpha - \omega_\beta)^2} \quad (20)$$

we obtained $k_{XZ} = 4.94 \times 10^{-12} \text{ ms}^{-1}$, $k_{YZ} = 6.20 \times 10^{-13} \text{ ms}^{-1}$, and $k_{XY} = 1.49 \times 10^{-10} \text{ ms}^{-1}$ at 300K and in the *p*-terphenyl host environment. This is because the fluctuations of ZFS are

extremely small compared to the vibrational energies, which should imply that the SLR can be adequately described within the framework of Fermi's golden rule based on second-order perturbation expansion. As a result, the contribution from case (1) can be negligible.

For case (2), using the second derivative terms in the Herzberg-Teller expansion of ZFS fluctuations,

$$\hat{H}_{\text{S-B}}(t) \approx \frac{1}{2} \sum_{\alpha} \left(\hat{\mathbf{S}}^{\top} \frac{\partial^2 \mathbf{D}}{\partial Q_{\alpha}^2} \hat{\mathbf{S}} \right) \otimes \hat{Q}_{\alpha}^2(t) + \sum_{\alpha < \beta} \left(\hat{\mathbf{S}}^{\top} \frac{\partial^2 \mathbf{D}}{\partial Q_{\alpha} \partial Q_{\beta}} \hat{\mathbf{S}} \right) \otimes \hat{Q}_{\alpha}(t) \hat{Q}_{\beta}(t), \quad (21)$$

SLR rate constants can be expressed as follows:

$$k_{ab} = \frac{2}{\hbar^2} \sum_{\alpha \leq \beta} \left(1 - \frac{\delta_{\alpha\beta}}{2} \right) |V_{ab}^{\alpha\beta}|^2 G_{\alpha\beta}(\omega_{ab}), \quad (22)$$

where $V_{ab}^{\alpha\beta} = \langle a | \hat{\mathbf{S}}^{\top} \frac{\partial^2 \mathbf{D}}{\partial Q_{\alpha} \partial Q_{\beta}} \hat{\mathbf{S}} | b \rangle$ and the spectral densities are

$$G_{\alpha\beta}(\omega) = \frac{\hbar}{4} \left[\frac{\Delta_{\alpha\beta}}{\Delta_{\alpha\beta}^2 + \hbar^2(\omega + \omega_{\alpha} + \omega_{\beta})^2} \bar{n}_{\alpha} \bar{n}_{\beta} + \frac{\Delta_{\alpha\beta}}{\Delta_{\alpha\beta}^2 + \hbar^2(\omega + \omega_{\alpha} - \omega_{\beta})^2} \bar{n}_{\alpha} (\bar{n}_{\beta} + 1) \right. \\ \left. + \frac{\Delta_{\alpha\beta}}{\Delta_{\alpha\beta}^2 + \hbar^2(\omega - \omega_{\alpha} + \omega_{\beta})^2} (\bar{n}_{\alpha} + 1) \bar{n}_{\beta} + \frac{\Delta_{\alpha\beta}}{\Delta_{\alpha\beta}^2 + \hbar^2(\omega - \omega_{\alpha} - \omega_{\beta})^2} (\bar{n}_{\alpha} + 1) (\bar{n}_{\beta} + 1) \right]. \quad (23)$$

Here, $\Delta_{\alpha\beta} = \Delta_{\alpha} + \Delta_{\beta}$, and if the summation index changes to $\alpha \neq \beta$, the factor $1 - \frac{\delta_{\alpha\beta}}{2}$ is replaced by $\frac{1}{2}$. Using the normal modes of *p*-terphenyl and RESP point charges for the D tensor calculation, Raman relaxation rate constants were computed by numerically differentiating the D tensor along dimensionless coordinates with displacements in the range [-0.05:0.05]. The results are presented in Table S3. Compared to the direct relaxation rates calculated from the first derivatives (discussed in the main text), the Raman relaxation rates are substantially larger. Notably, the calculated value of k_{XY} greatly exceeds the experimental value of 4ms^{-1} . A mode-resolved analysis revealed that second-derivative terms corresponding to diagonal components ($\alpha = \beta$) contribute most significantly. Figure S3 shows heatmaps of the spin-phonon coupling values for each pair of vibrational modes. It

is evident from this figure that diagonal components tend to be larger than off-diagonal ones. Also, the number of modes with large coupling contributions increases in the order of XZ, YZ, and XY, which likely explains the computed trend in the SLR rate constants. In addition, as shown in Figure S4, the spectral density exhibits exponentially large values in the region where low-frequency modes are involved. This is likely because the phonon population becomes large below thermal energies 209cm^{-1} . Therefore, the contribution to the Raman relaxation rate constant tends to be large when low-frequency modes are involved and the coupling corresponds to diagonal components with $\alpha = \beta$.

Finally, it should be noted that this calculation is highly sensitive to the accuracy of the D tensor, making it difficult to obtain reliable results. Let us consider the second derivative of the D tensor along the Q_1 normal mode, which gives the largest contributions to k_{YZ} and k_{XY} . The second derivative is numerically calculated as follows:

$$\left. \frac{\partial^2 \mathbf{D}(\mathbf{Q})}{\partial Q_\alpha^2} \right|_{\mathbf{Q}^{(0)}} \approx \frac{\mathbf{D}(\cdots, Q_\alpha^{(0)} + \delta Q_\alpha, \cdots) + \mathbf{D}(\cdots, Q_\alpha^{(0)} - \delta Q_\alpha, \cdots) - 2\mathbf{D}(\mathbf{Q}^{(0)})}{(\delta Q_\alpha)^2}, \quad (24)$$

and calculated D tensors with $\delta Q_1 = 0.05$ were

$$\mathbf{D}(\mathbf{Q}^{(0)})/\text{cm}^{-1} = \begin{pmatrix} -0.013743 & 0. & 0. \\ 0. & -0.011242 & 0. \\ 0. & 0. & 0.024985 \end{pmatrix}, \quad (25)$$

$$\mathbf{D}(Q_1^{(0)} + \delta Q_1, \dots)/\text{cm}^{-1} = \begin{pmatrix} -0.013743 & 0.000002 & -0.000001 \\ 0.000002 & -0.011241 & 0.000001 \\ -0.000001 & 0.000001 & 0.024984 \end{pmatrix}, \quad (26)$$

$$\mathbf{D}(Q_1^{(0)} - \delta Q_1, \dots)/\text{cm}^{-1} = \begin{pmatrix} -0.013744 & 0.000002 & 0. \\ 0.000002 & -0.011241 & 0. \\ 0. & 0. & 0.024984 \end{pmatrix}, \quad (27)$$

$$\left. \frac{\partial^2 \mathbf{D}(\mathbf{Q})}{\partial Q_1^2} \right|_{\mathbf{Q}^{(0)}} / \text{cm}^{-1} = \begin{pmatrix} -0.000058 & 0.001858 & -0.000132 \\ 0.001858 & 0.00071 & 0.000619 \\ -0.000132 & 0.000619 & -0.000652 \end{pmatrix}. \quad (28)$$

Within the current model, even a small difference 10^{-6}cm^{-1} in the D tensor can lead to significant changes in the calculated SLR rate constants. To accurately evaluate Raman relaxation, the D tensor must be computed with very high precision. In particular, higher-order derivatives demand greater precision, and numerical differentiation appears to be insufficient for such a task. Also, the construction of the spectral density has a substantial impact on the rate constants. Therefore, given the small fluctuations in the D tensor originating from electron spin–spin coupling, it is difficult to quantitatively evaluate higher-order phonon processes using numerical derivatives based on the Taylor expansion approach of the ZFS Hamiltonian. For a more accurate treatment, it may be preferable to compute fluctuations without relying on the Herzberg-Teller expansions, such as molecular dynamics or similar approaches.

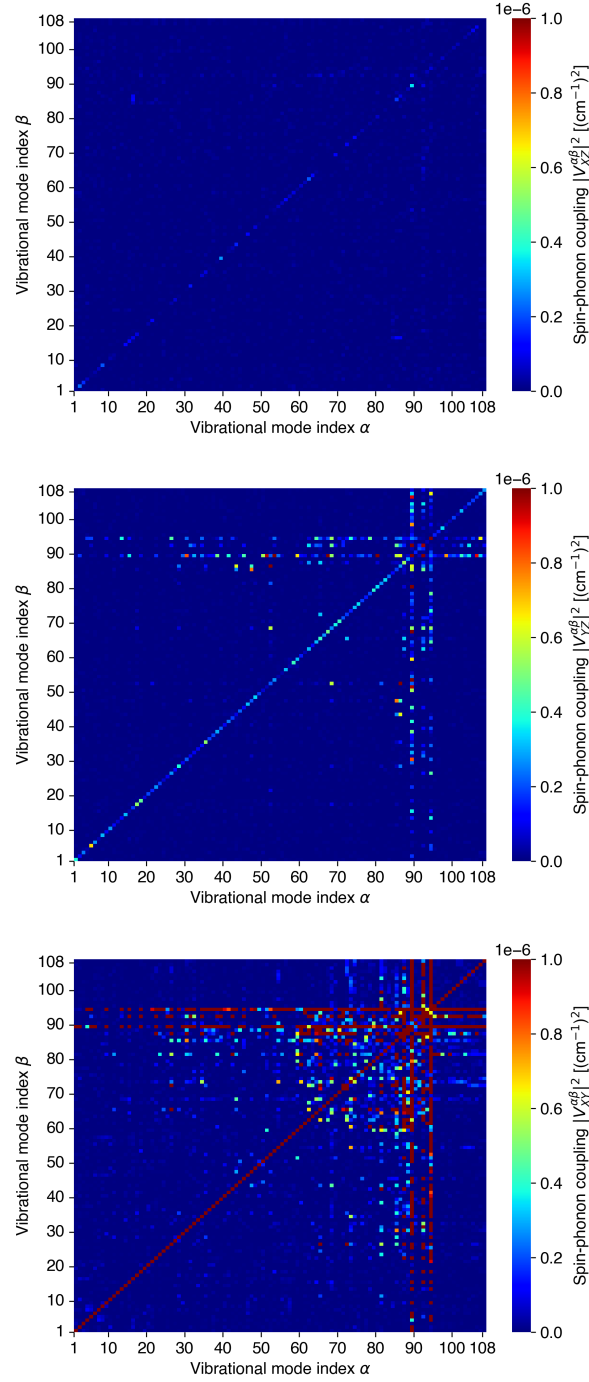


Figure S3: Heatmaps of the spin-phonon coupling derived from the second derivatives of the D tensor along vibrational modes. From top to bottom, the panels correspond to couplings associated with transitions between $X \leftrightarrow Z$, $Y \leftrightarrow Z$, and $X \leftrightarrow Y$ spin sublevels, respectively. For clarity, the upper limit of the color bar was set to $10^{-6}(\text{cm}^{-1})^2$.

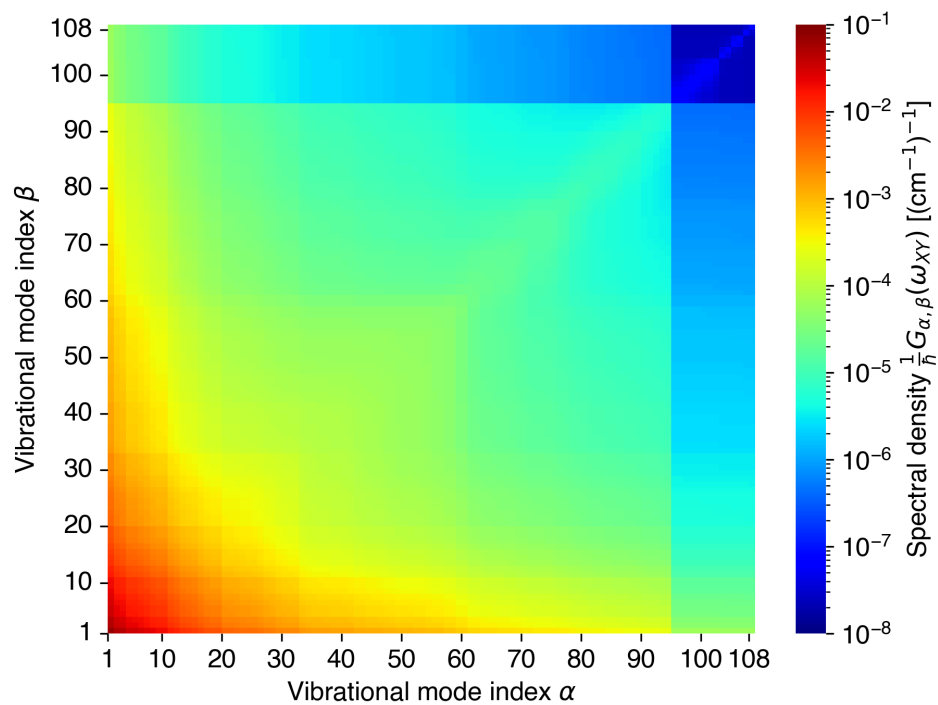


Figure S4: Heatmap of the spectral density for Raman relaxation evaluated at 300K and at the energy corresponding to ω_{XY} , for each pair of vibrational modes used in the second derivative of the D tensor.

Table S3: Table of Raman relaxation rate constants calculated from the second derivatives of the D tensor. The indices α and β correspond to the vibrational modes involved in the differentiation.

k_{XZ}		k_{YZ}		k_{XY}	
$Q_{\alpha,\beta}(\omega_\alpha, \omega_\beta/\text{cm}^{-1})$	$k_{XZ}^{(\alpha,\beta)}/\text{ms}^{-1}$	$Q_{\alpha,\beta}(\omega_\alpha, \omega_\beta/\text{cm}^{-1})$	$k_{YZ}^{(\alpha,\beta)}/\text{ms}^{-1}$	$Q_{\alpha,\beta}(\omega_\alpha, \omega_\beta/\text{cm}^{-1})$	$k_{XY}^{(\alpha,\beta)}/\text{ms}^{-1}$
Total	5.64	Total	13.58	Total	363.78
$Q_{2,2}(55,55)$	1.44	$Q_{1,1}(38,38)$	5.22	$Q_{1,1}(38,38)$	47.01
$Q_{3,3}(60,60)$	0.88	$Q_{5,5}(81,81)$	1.91	$Q_{5,5}(81,81)$	31.30
$Q_{8,8}(119,119)$	0.27	$Q_{3,3}(60,60)$	1.28	$Q_{2,2}(55,55)$	29.09
$Q_{1,3}(38,60)$	0.25	$Q_{2,2}(55,55)$	0.67	$Q_{4,4}(80,80)$	28.35

7 Supplementary Figures

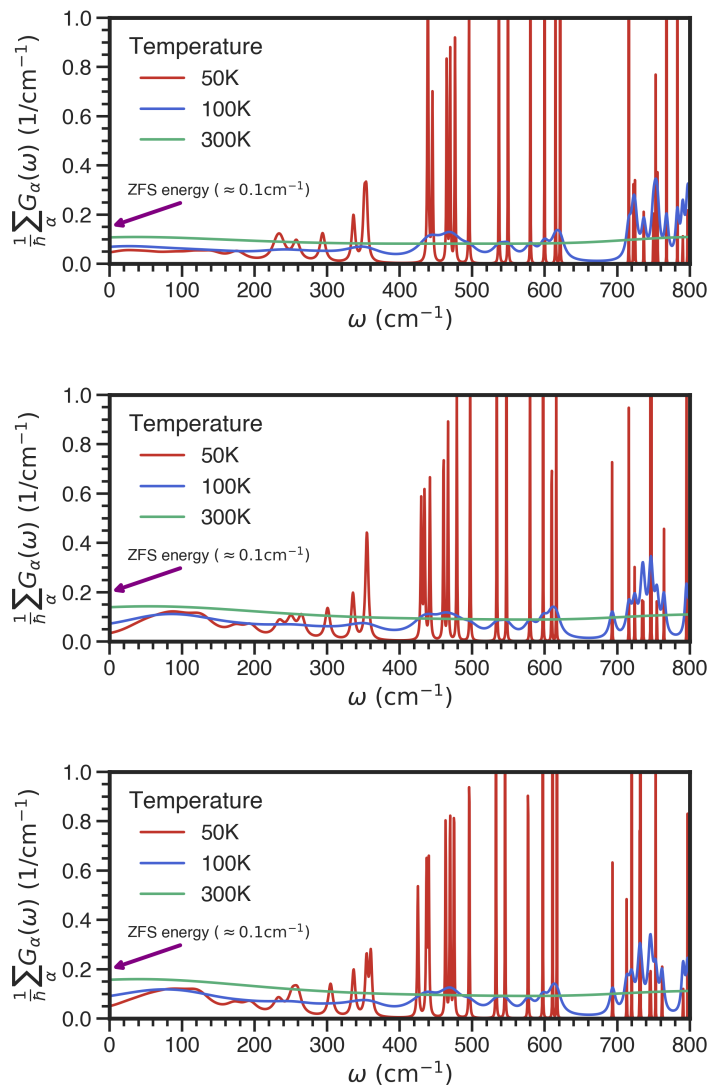


Figure S5: The plots of the spectral density of pentacene in vacuum (top), *p*-terphenyl (middle), and benzoic acid (bottom) as a function of the energy difference between the transitioning levels. Since the ZFS energy is much smaller than the vibrational energy, only the components near the origin are considered when evaluating the SLR (purple arrow).

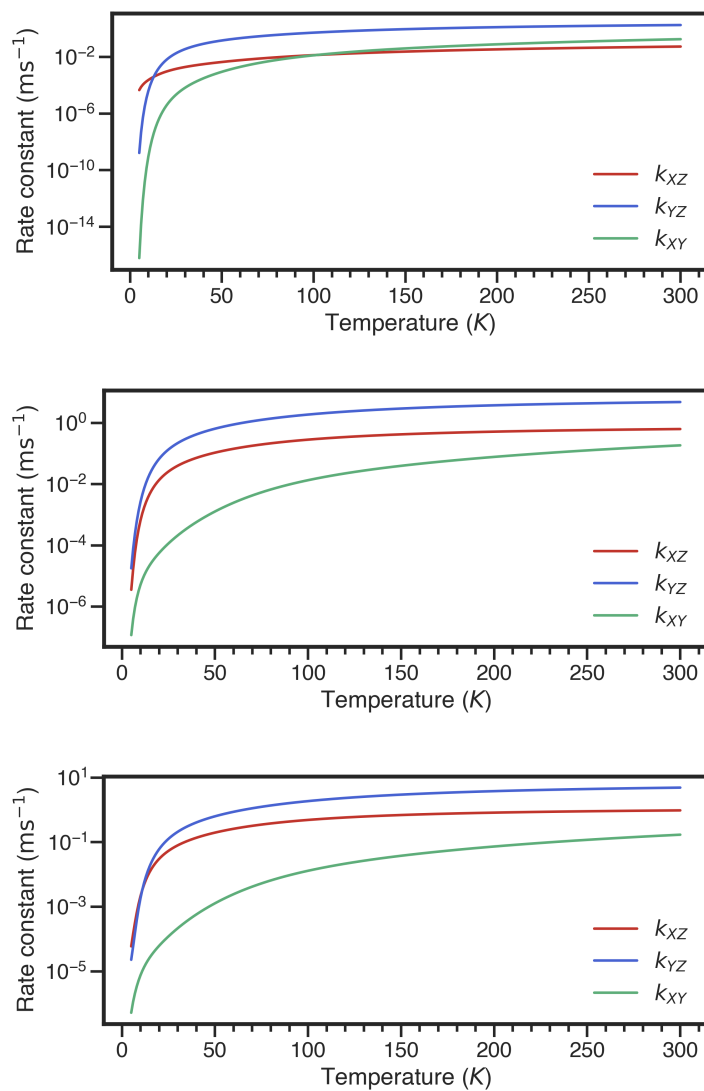


Figure S6: Temperature dependence of the SLR rate constants of pentacene in vacuum (top), *p*-terphenyl (middle), and benzoic acid (bottom) under zero magnetic field.

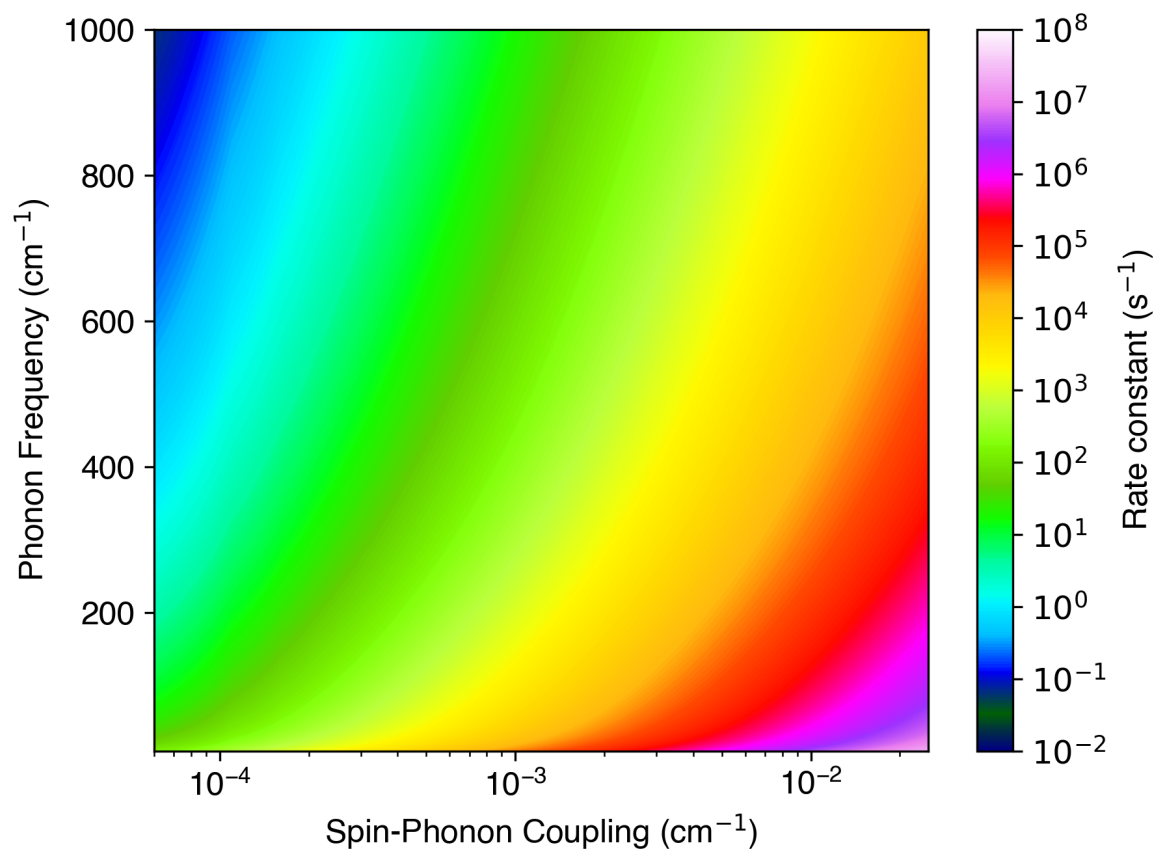


Figure S7: The plot of the SLR rate constants at 300K with respect to phonon frequencies and spin-phonon couplings, i.e., the derivative values of the D tensor. The energy difference between the transitioning levels is 0.05cm⁻¹.

8 Values of the Derivatives of D Tensors Used in This Study

Symmetry-broken solutions in CASSCF may or may not arise depending on factors such as the numerical stability of the SCF algorithm and molecular geometry. To ensure reproducibility, the derivative values of the D tensor along normal modes used in this study are provided below. All units are cm^{-1} , and the ZFS principal axis coordinate system is used. Values smaller than 5×10^{-5} are displayed as 0.

8.1 Naphthalene

i	freq.	Dxx	Dyy	Dzz	Dxy	Dxz	Dyz
1	146	0	0	0	0	0	0
2	151	0	0	0	0	0	0
3	283	0	0	0	0	-0.0037	0
4	351	0	0	0	0	0	0
5	402	0	0	0	0	0	0
6	457	0	0	0	0	0	0.0020
7	482	0	0	0	0.0074	0	0
8	498	-0.0009	0.0013	-0.0005	0	0	0
9	516	0	0	0	0	0	0
10	585	0	0	0	0	0	0
11	664	0	0	0	0	-0.0014	0
12	671	0	0	0	0	0	0
13	719	0	0	0	0	0	0
14	734	0	0	0	0	0	-0.0020
15	752	0.0016	-0.0011	-0.0005	0	0	0
16	779	0	0	0	0	0.0038	0
17	790	0	0	0	0	0	0
18	807	0	0	0	0	0	0
19	896	0	0	0	0	0	-0.0002
20	899	0	0	0	0	0	0
21	907	0	0	0	0.0017	0	0
22	929	0	0	0	0	0	0
23	955	0	0	0	0	0	0.0037
24	975	0	0	0	-0.0180	0	0
25	1036	0.0009	0.0002	-0.0011	0	0	0
26	1046	0	0	0	0	0	0
27	1121	0	0	0	0	0	0
28	1146	0.0025	-0.0013	-0.0011	0	0	0
29	1163	0	0	0	0	0	0
30	1198	0	0	0	-0.0048	0	0
31	1257	0	0	0	0	0	0
32	1355	0	0	0	-0.0154	0	0
33	1374	0.0062	-0.0003	-0.0059	0	0	0
34	1377	0	0	0	0	0	0
35	1404	0	0	0	0.0043	0	0
36	1440	0	0	0	0	0	0
37	1445	-0.0002	0.0007	-0.0004	0	0	0
38	1448	0	0	0	0	0	0
39	1505	0	0	0	0	0	0
40	1604	-0.0108	0.0053	0.0056	0	0	0
41	3099	0	0	0	-0.0001	0	0
42	3100	0	0	0	0	0	0

43	3104	-0.0013	0.0008	0.0005	0	0	0
44	3105	0	0	0	0	0	0
45	3116	0	0	0	0.0010	0	0
46	3117	0	0	0	0	0	0
47	3131	0	0	0	0	0	0
48	3132	0.0004	-0.0004	0	0	0	0

8.2 Anthracene

i	freq.	Dxx	Dyy	Dzz	Dxy	Dxz	Dyz
1	73	0	0	0	0	0	0
2	96	0	0	0	0	0	0
3	226	0	0	0	0	0.0010	0
4	228	0	0	0	0	0	0
5	250	0	0	0	0	0	0.0009
6	328	0	0	0	0	0	0
7	376	0	0	0	0.0017	0	0
8	385	-0.0001	0.0003	-0.0002	0	0	0
9	432	0	0	0	0	0	0
10	443	0	0	0	0	0.0015	0
11	509	0	0	0	0	0	0
12	517	0	0	0	0.0033	0	0
13	545	0	0	0	0	0	-0.0004
14	599	0	0	0	0	0	0
15	602	-0.0003	-0.0003	0.0006	0	0	0
16	662	0	0	0	0	0	0
17	698	0	0	0	0	0	0
18	706	0	0	0	0	0.0005	0
19	723	0	0	0	0	0	-0.0006
20	747	-0.0005	0.0002	0.0003	0	0	0
21	769	0	0	0	0	0	0
22	779	0	0	0	0	0	0
23	802	0	0	0	0	0	0.0005
24	818	0	0	0	0	0	0
25	868	0	0	0	0	0.0017	0
26	870	0	0	0	0	0	0
27	876	0	0	0	0	0	0
28	888	0	0	0	0	0	0
29	897	0	0	0	-0.0029	0	0
30	904	0	0	0	0	0	0.0002
31	906	0	0	0	0	0	0
32	978	0	0	0	0	0	-0.0030
33	1023	0	0	0	0	0	0
34	1030	-0.0005	0.0004	0	0	0	0
35	1067	0	0	0	-0.0040	0	0
36	1096	0	0	0	0	0	0
37	1132	0	0	0	0	0	0
38	1149	0.0019	-0.0009	-0.0010	0	0	0
39	1162	0	0	0	-0.0043	0	0
40	1168	0	0	0	0	0	0
41	1195	0.0025	-0.0013	-0.0011	0	0	0
42	1248	0	0	0	-0.0002	0	0
43	1250	0	0	0	-0.0018	0	0
44	1265	0	0	0	0	0	0
45	1271	0	0	0	0	0	0
46	1379	0	0	0	0.0032	0	0
47	1393	-0.0049	0.0005	0.0045	0	0	0
48	1432	0	0	0	0	0	0
49	1438	0	0	0	0	0	0
50	1444	0	0	0	0	0	0
51	1447	0	0	0	0.0087	0	0
52	1486	0.0054	-0.0022	-0.0032	0	0	0
53	1494	0	0	0	-0.0034	0	0
54	1548	0	0	0	0	0	0

55	1550	0	0	0	0	0	0
56	1580	0.0063	-0.0038	-0.0025	0	0	0
57	3089	0	0	0	0	0	0
58	3090	0.0006	-0.0002	-0.0004	0	0	0
59	3095	-0.0003	0.0002	0.0001	0	0	0
60	3095	0	0	0	0	0	0
61	3097	0.0005	-0.0004	-0.0002	0	0	0
62	3098	0	0	0	0	0	0
63	3114	0	0	0	-0.0003	0	0
64	3115	0	0	0	0	0	0
65	3129	0	0	0	0	0	0
66	3129	-0.0003	0.0002	0	0	0	0

8.3 Tetracene

i	freq.	Dxx	Dyy	Dzz	Dxy	Dxz	Dyz
1	40	0	0	0	0	0	-0.0001
2	70	0	0	0	0	0	0
3	133	0	0	0	0	-0.0001	0
4	160	0	0	0	0	0	0
5	184	0	0	0	0	0	-0.0009
6	268	0	0	0	0	0	0
7	293	0	0	0	0.0003	0	0
8	305	0	0	0	0	0	0
9	310	0.0001	0	0	0	0	0
10	348	0	0	0	0	-0.0004	0
11	430	0	0	0	0	0	0
12	436	0	0	0	0	0	0
13	449	0	0	0	0	0	0
14	464	0	0	0	0	0.0009	0
15	491	0	0	0	0.0039	0	0
16	530	0	0	0	0	0	0.0002
17	543	0	0	0	0	0	0
18	552	0	0	0	0	0	0
19	610	0	0	0	0	0	0
20	617	-0.0008	0.0001	0.0006	0	0	0
21	620	0	0	0	0	0	0
22	715	0	0	0	0	-0.0001	0
23	718	0	0	0	0	0	0
24	739	0	0	0	0	0	-0.0001
25	750	-0.0002	-0.0003	0.0005	0	0	0
26	757	0	0	0	0	0	0.0004
27	764	0	0	0	0	0	0
28	776	0	0	0	0.0042	0	0
29	777	0	0	0	0	0.0001	-0.0002
30	795	0	0	0	0	-0.0006	0
31	801	0	0	0	0	0.0001	0
32	840	0	0	0	0	0	0
33	850	0	0	0	0	0	-0.0001
34	863	-0.0002	0.0001	0.0001	0	0	0
35	882	0	0	0	-0.0014	0	0
36	895	0	0	0	0	0.0005	0
37	896	0	0	0	0	0	0
38	900	0	0	0	0	0	0
39	917	0	0	0	0	0	0
40	918	0	0	0	0	0	0
41	922	0	0	0	0	0	0
42	985	0	0	0	0	0	-0.0024
43	1034	0	-0.0001	0.0001	0	0	0
44	1035	0	0	0	0	0	0
45	1104	0	0	0	0	0	0
46	1105	0	0	0	-0.0095	0	0
47	1133	0	0	0	0	0	0
48	1148	0.0014	-0.0006	-0.0008	0	0	0

49	1153	0	0	0	-0.0056	0	0
50	1164	0	0	0	0	0	0
51	1198	-0.0020	0.0010	0.0010	0	0	0
52	1203	0	0	0	0	0	0
53	1233	0	0	0	0	0	0
54	1248	0	0	0	-0.0007	0	0
55	1251	0	0	0	0	0	0
56	1279	0	0	0	0	0	0
57	1285	0	0	0	0	0	0
58	1290	0	0	0	-0.0016	0	0
59	1346	0.0006	0.0004	-0.0009	0	0	0
60	1390	0	0	0	0	0	0
61	1404	0.0039	-0.0008	-0.0031	0	0	0
62	1430	0.0004	-0.0003	-0.0001	0	0	0
63	1436	0	0	0	0	0	0
64	1442	0	0	0	-0.0061	0	0
65	1460	0	0	0	0	0	0
66	1481	0	0	0	-0.0123	0	0
67	1503	0.0038	-0.0023	-0.0016	0	0	0
68	1506	-0.0001	0.0001	0.0001	0	0	0
69	1553	0	0	0	0	0	0
70	1570	-0.0033	0.0024	0.0009	0	0	0
71	1581	0	0	0	0.0006	0	0
72	1582	0	0	0	-0.0135	0	0
73	3083	0	0	0	0	0	0
74	3083	0	0	0	-0.0001	0	0
75	3086	0.0005	-0.0002	-0.0002	0	0	0
76	3089	0	0	0	0	0	0
77	3095	0	0	0	-0.0002	0	0
78	3096	0	0	0	0	0	0
79	3098	0	0	0	0	0	0
80	3098	0.0001	-0.0001	0	0	0	0
81	3114	0	0	0	0.0019	0	0
82	3114	0	0	0	-0.0001	0	0
83	3127	0	0	0	0	0	0
84	3128	0	0	0	0	0	0

8.4 Pentacene

i	freq.	Dxx	Dyy	Dzz	Dxy	Dxz	Dyz
1	21	0	0	0	0	0	0
2	53	0	0	0	0	0	0
3	89	0	0	0	0	0.0001	0
4	117	0	0	0	0	0	0
5	141	0	0	0	0	0	0.0009
6	176	0	0	0	0	0	0
7	231	0	0	0	-0.0001	0	0
8	236	0	0	0	0	0	0
9	258	-0.0003	0.0003	0	0	0	0
10	294	0	0	0	0	-0.0002	0
11	336	0	0	0	0	0	-0.0008
12	351	0	0	0	0	0	0
13	354	0	0	0	0	0	0
14	439	0	0	0	0.0001	0	0
15	439	0	0	0	0.0004	0	0
16	445	0	0	0	0	-0.0001	0
17	465	0	0	0	0	0.0002	0
18	470	0	0	0	0	0	0
19	476	0	0	0	0	0	0
20	496	0	0	0	0.0007	0	0
21	537	0	0	0	0	0	0
22	549	0	0	0	0	0	-0.0002
23	580	0	0	0	0	0	0
24	600	-0.0001	0.0005	-0.0005	0	0	0

25	615	0.0001	0.0001	-0.0002	0	0	0
26	621	0	0	0	0	0	0
27	716	0	0	0	0.0005	0	0
28	722	0	0	0	0	0	0
29	725	0	0	0	0	0.0001	0
30	737	0	0	0	0	0	0.0003
31	750	-0.0001	-0.0003	0.0005	0	0	0
32	753	0	0	0	0	0	0
33	756	0	0	0	0	0	0
34	768	0	0	0	0	0	0
35	783	0	0	0	0	0	0.0003
36	790	0	0	0	0	0	0
37	797	0.0005	-0.0003	-0.0002	0	0	0
38	800	0	0	0	0	0	-0.0004
39	825	0	0	0	0	0	0
40	837	0	0	0	0	0	0
41	843	0	0	0	0	-0.0001	0
42	863	0	0	0	0	0	0
43	869	0	0	0	0	0	-0.0003
44	880	0	0	0	0	0	0
45	899	0	0	0	0	0	0
46	909	0	0	0	0	0.0002	0
47	909	0	0	0	0	0	0
48	914	0	0	0	-0.0002	0	0
49	920	0	0	0	0	0	0
50	926	0	0	0	0	0	0.0001
51	928	0	0	0	0	0	0
52	981	0	0	0	0	0	0.0014
53	1030	0	0	0	0	0	0
54	1030	-0.0003	0.0002	0.0001	0	0	0
55	1108	0	0	0	0	0	0
56	1117	0	0	0	0.0002	0	0
57	1128	0	0	0	0	0	0
58	1147	0.0004	-0.0001	-0.0003	0	0	0
59	1154	0	0	0	-0.0011	0	0
60	1160	0	0	0	0	0	0
61	1173	0	0	0	0	0	0
62	1180	0.0019	-0.0013	-0.0006	0	0	0
63	1197	0	0	0	0	0	0
64	1238	0	0	0	-0.0002	0	0
65	1252	0	0	0	0	0	0
66	1254	0	0	0	0.0002	0	0
67	1264	0	0	0	0.0007	0	0
68	1266	0.0010	-0.0012	0.0002	0	0	0
69	1290	0	0	0	0	0	0
70	1299	0	0	0	0	0	0
71	1320	0	0	0	0	0	0
72	1361	-0.0012	0.0011	0.0001	0	0	0
73	1378	0	0	0	0	0	0
74	1395	0	0	0	-0.0004	0	0
75	1412	-0.0017	0.0005	0.0012	0	0	0
76	1423	0	0	0	0	0	0
77	1432	0	0	0	0	0	0
78	1446	0	0	0	0	0	0
79	1463	-0.0027	0.0021	0.0006	0	0	0
80	1481	0	0	0	0	0	0
81	1492	0	0	0	-0.0025	0	0
82	1506	0.0025	-0.0019	-0.0006	0	0	0
83	1512	0	0	0	-0.0001	0	0
84	1556	0	0	0	0	0	0
85	1565	0.0010	-0.0007	-0.0003	0	0	0
86	1577	0	0	0	0	0	0
87	1600	0	0	0	0	0	0
88	1607	0	0	0	0.0004	0	0
89	3083	0	0	0	0	0	0
90	3083	0.0001	-0.0001	0	0	0	0
91	3084	0	0	0	0	0	0

92	3084	0	0	0	0	0	0
93	3089	-0.0004	0.0002	0.0002	0	0	0
94	3090	0	0	0	0	0	0
95	3095	0	0	0	0	0	0
96	3096	0	0	0	0	0	0
97	3098	0	0	0	0	0	0
98	3098	0	0	0	0	0	0
99	3115	0	0	0	0	0	0
100	3115	0	0	0	0	0	0
101	3127	0	0	0	0	0	0
102	3127	0	0.0001	0	0	0	0

8.5 DAT

i	freq.	Dxx	Dyy	Dzz	Dxy	Dxz	Dyz
1	46	0	0	0	0	0.0002	0
2	68	0	0	0	0	0	-0.0002
3	140	0	0	0	0	0.0001	0
4	169	0	0	0	-0.0001	0	0
5	184	0	0	0	0	0	-0.0010
6	277	0	0	0	0	0	0
7	306	0	0	0	-0.0006	0	0
8	307	0	0	0	0	0	-0.0002
9	320	0.0001	0	-0.0001	0	0	0
10	364	0	0	0	0	-0.0004	0
11	434	0	0	0	0	-0.0003	0
12	455	0	0	0	0	0.0002	0
13	468	0	0	0	-0.0010	0	0
14	477	0	0	0	0	-0.0010	0
15	492	0	0	0	0.0025	0	0
16	528	0	0	0	0	0	0.0002
17	551	0.0002	-0.0001	-0.0001	0	0	0
18	553	0	0	0	0	0	0
19	594	-0.0004	0.0002	0.0002	0	0	0
20	611	-0.0008	0.0001	0.0007	0	0	0
21	625	0	0	0	-0.0003	0	0
22	724	0	0	0	0	0	0
23	729	0	0	0	0	0	-0.0001
24	733	-0.0001	-0.0003	0.0004	0	0	0
25	743	0	0	0	0	-0.0002	0
26	764	-0.0002	-0.0001	0.0002	0	0	0
27	776	0	0	0	0	0	0.0002
28	780	0	0	0	0.0021	0	0
29	783	0	0	0	0	0	0.0005
30	847	0	0	0	0	0	0.0007
31	849	0	0	0	0	-0.0005	0
32	874	0	0	0	0	0	-0.0008
33	880	0	0	0	0.0012	0	0
34	881	0.0005	-0.0003	-0.0002	0	0	0
35	912	0	0	0	0	-0.0005	0
36	926	0	0	0	0	0.0003	0
37	926	0	0	0	0.0003	0	0
38	930	0	0	0	0	0	0.0008
39	934	0	0	0	0	0	-0.0001
40	947	0	0	0	0	0	0.0020
41	1025	0.0002	-0.0001	-0.0001	0	0	0
42	1034	-0.0002	0	0.0002	0	0	0
43	1101	0	0	0	-0.0027	0	0
44	1103	0	0	0	0.0006	0	0
45	1132	0.0003	-0.0002	-0.0001	0	0	0
46	1148	-0.0016	0.0007	0.0009	0	0	0
47	1168	0	0	0	-0.0022	0	0
48	1172	-0.0011	0.0006	0.0005	0	0	0
49	1219	0	0	0	0.0007	0	0

50	1239	-0.0014	0.0007	0.0007	0	0	0
51	1243	0	0	0	0.0019	0	0
52	1271	0	0	0	0.0012	0	0
53	1273	0.0025	-0.0010	-0.0015	0	0	0
54	1296	0	0	0	-0.0009	0	0
55	1314	0.0010	-0.0007	-0.0003	0	0	0
56	1350	0.0015	0.0001	-0.0016	0	0	0
57	1376	0	0	0	0.0043	0	0
58	1391	-0.0023	0.0001	0.0021	0	0	0
59	1406	0	0	0	0.0051	0	0
60	1422	-0.0020	0.0004	0.0015	0	0	0
61	1449	0.0004	-0.0003	-0.0001	0	0	0
62	1452	0	0	0	0.0008	0	0
63	1492	-0.0040	0.0023	0.0018	0	0	0
64	1505	0	0	0	-0.0025	0	0
65	1549	0.0005	-0.0004	-0.0001	0	0	0
66	1567	-0.0001	0	0	0.0034	0	0
67	1570	-0.0035	0.0025	0.0010	0	0	0
68	1596	0	0	0	0.0018	0	0
69	3101	0	0	0	0	0	0
70	3104	0	0	0	0	0	0
71	3108	0	0	0	0.0001	0	0
72	3108	0	0	0	0.0001	0	0
73	3109	0.0004	-0.0002	-0.0002	0	0	0
74	3117	0	0	0	0.0005	0	0
75	3117	0	0	0	0	0	0
76	3125	0	0	0	0.0003	0	0
77	3130	0	0	0	0	0	0
78	3132	0	0	0	0	0	0

8.6 TrAT1

i	freq.	Dxx	Dyy	Dzz	Dxy	Dxz	Dyz
1	29	0	0	0	0	0.0002	0.0002
2	47	0	0	0	0	0.0001	-0.0011
3	134	0	0	0	0	0	0
4	170	0	0	0	0	0.0002	-0.0011
5	172	-0.0001	0.0001	0	0.0003	0	0
6	275	0	0	0	0	0	-0.0001
7	299	0	0	0	0	0	0.0003
8	311	-0.0003	0.0003	0	0.0008	0	0
9	321	0.0001	-0.0001	0	-0.0003	0	0
10	363	0	0	0	0	-0.0004	-0.0001
11	432	0	0	0	0	0.0003	0
12	455	0	0	0	0	0.0003	0.0001
13	482	0	0	0	0	0.0011	0.0001
14	483	0.0001	-0.0001	0	-0.0001	0	0
15	499	0.0008	-0.0008	0	-0.0025	0	0
16	523	0	0	0	0	0	-0.0003
17	549	0	0	0	0	0.0001	0.0001
18	558	-0.0001	0.0001	0	0	0	0
19	587	-0.0005	0.0002	0.0003	-0.0001	0	0
20	608	0.0009	-0.0001	-0.0008	0.0001	0	0
21	637	0	0.0001	-0.0001	0.0002	0	0
22	711	0	0	0	0	0	0
23	729	0	-0.0003	0.0004	-0.0001	0	0
24	733	0	0	0	0	0.0001	0
25	756	0	0	0	0	0.0002	-0.0001
26	764	-0.0003	0	0.0003	0	0	0
27	782	0	0	0	0	0	0.0001
28	786	0.0005	-0.0005	0	-0.0015	0	0
29	820	0	0	0	0	-0.0002	0.0005
30	849	0	0	0	0	0.0004	-0.0007
31	851	0	0	0	0	-0.0003	-0.0004

32	884	0	0.0001	-0.0002	0.0010	0	0
33	889	0.0009	-0.0007	-0.0002	-0.0009	0	0
34	912	0	0	0	0	0.0005	0
35	916	0	0	0	0	-0.0002	-0.0002
36	925	0	0	0	0	-0.0001	0.0007
37	930	0.0001	-0.0001	0	0.0001	0	0
38	941	0	0	0	0	0	0
39	954	0	0	0	0	-0.0003	0.0022
40	1034	0.0003	-0.0001	-0.0003	0	0	0
41	1049	-0.0002	0	0.0001	-0.0002	0	0
42	1099	0.0009	-0.0005	-0.0004	-0.0008	0	0
43	1101	0.0007	-0.0008	0.0001	-0.0028	0	0
44	1148	0.0015	-0.0007	-0.0008	0	0	0
45	1168	-0.0008	0.0008	0	0.0018	0	0
46	1174	0.0008	-0.0005	-0.0004	0.0002	0	0
47	1208	-0.0004	0	0.0003	-0.0012	0	0
48	1236	0.0008	-0.0009	0.0001	-0.0025	0	0
49	1253	-0.0010	0.0004	0.0007	-0.0005	0	0
50	1267	0	-0.0003	0.0004	-0.0011	0	0
51	1288	0.0006	-0.0007	0.0001	-0.0009	0	0
52	1303	0.0003	-0.0004	0.0001	-0.0012	0	0
53	1314	-0.0043	0.0021	0.0022	-0.0001	0	0
54	1334	-0.0017	-0.0002	0.0020	-0.0006	0	0
55	1357	0.0017	0	-0.0017	0.0017	0	0
56	1387	0.0009	-0.0005	-0.0004	-0.0014	0	0
57	1407	0.0031	-0.0017	-0.0014	-0.0043	0	0
58	1418	-0.0009	-0.0007	0.0016	-0.0026	0	0
59	1438	-0.0010	0.0007	0.0002	0.0011	0	0
60	1451	0.0003	-0.0003	0	-0.0011	0	0
61	1487	0.0040	-0.0023	-0.0017	0.0001	0	0
62	1501	0.0004	0	-0.0004	0.0016	0	0
63	1540	0.0015	-0.0009	-0.0006	0.0004	0	0
64	1562	0.0012	-0.0012	0	-0.0037	0	0
65	1567	0.0033	-0.0022	-0.0011	0.0009	0	0
66	1585	0.0014	-0.0008	-0.0006	0.0001	0	0
67	3080	-0.0001	0.0001	0	0	0	0
68	3102	0	0	0	0	0	0
69	3105	0	0	0	0	0	0
70	3108	0.0003	-0.0002	-0.0002	0.0001	0	0
71	3111	0.0004	-0.0002	-0.0002	0	0	0
72	3118	0	0	0	0	0	0
73	3119	0.0001	-0.0001	0	-0.0004	0	0
74	3131	0	0	-0.0001	0	0	0
75	3132	0	0	0	0	0	0

8.7 TrAT2

i	freq.	Dxx	Dyy	Dzz	Dxy	Dxz	Dyz
1	42	0	0	0	0	0.0002	-0.0001
2	61	0	0	0	0	0	-0.0003
3	137	0	0	0	0	0.0001	0
4	169	0	0.0001	-0.0001	0.0003	0	0
5	181	0	0	0	0	-0.0001	0.0010
6	273	0	0	0	0	0	0.0001
7	302	0	0	0	0	0	0.0003
8	306	0.0002	-0.0002	-0.0001	-0.0006	0	0
9	319	0.0002	0	-0.0001	0	0	0
10	353	0	0	0	0	0.0003	0.0001
11	432	0	0	0	0	-0.0004	-0.0001
12	445	0	0	0	0	0	0.0001
13	467	0.0002	-0.0002	-0.0001	-0.0010	0	0
14	473	0	0	0	0	-0.0010	0
15	495	-0.0008	0.0005	0.0003	0.0023	0	0
16	531	0	0	0	0	0.0001	0.0002

17	555	0.0004	-0.0002	-0.0002	-0.0002	0	0
18	574	0	0	0	0	-0.0001	-0.0002
19	599	0.0001	-0.0001	0.0001	0.0002	0	0
20	615	-0.0008	0.0001	0.0007	-0.0005	0	0
21	637	0.0005	-0.0001	-0.0004	-0.0001	0	0
22	726	0	0	0	0	0	0
23	733	0	0	0	0	0.0001	0.0001
24	739	0.0003	0.0002	-0.0005	-0.0002	0	0
25	771	0.0001	0	-0.0002	0	0	0
26	779	0	0	0	0	0	0
27	780	0.0004	-0.0003	-0.0001	-0.0017	0	0
28	790	0	0	0	0	-0.0001	0.0005
29	822	0	0	0	0	0.0002	0.0002
30	850	0	0	0	0	0	-0.0008
31	853	0	0	0	0	-0.0005	0
32	880	0.0008	-0.0005	-0.0002	-0.0007	0	0
33	886	0.0001	0	-0.0001	0.0008	0	0
34	916	0	0	0	0	0.0005	0.0001
35	922	0	0	0	0	0.0003	-0.0006
36	927	-0.0001	0.0001	0	-0.0004	0	0
37	935	0	0	0	0	-0.0001	0.0010
38	950	0	0	0	0	0.0002	-0.0019
39	955	0	0	0	0	0.0002	0.0001
40	1034	0.0002	0	-0.0002	-0.0001	0	0
41	1035	0.0005	-0.0002	-0.0003	-0.0003	0	0
42	1103	0.0004	-0.0005	0.0001	-0.0032	0	0
43	1146	-0.0008	0.0003	0.0004	-0.0004	0	0
44	1169	-0.0021	0.0009	0.0011	0.0006	0	0
45	1170	0	-0.0001	0.0001	-0.0018	0	0
46	1177	0.0004	-0.0001	-0.0003	-0.0007	0	0
47	1226	0.0005	-0.0002	-0.0003	-0.0006	0	0
48	1241	-0.0015	0.0005	0.0010	-0.0016	0	0
49	1247	0.0013	-0.0008	-0.0005	-0.0013	0	0
50	1260	0	-0.0003	0.0003	-0.0005	0	0
51	1273	0	0	0	0.0010	0	0
52	1298	0.0038	-0.0017	-0.0022	0.0009	0	0
53	1302	-0.0013	0.0006	0.0007	0.0007	0	0
54	1339	0.0026	-0.0002	-0.0024	0.0010	0	0
55	1374	-0.0014	0.0005	0.0009	0.0016	0	0
56	1386	0.0023	-0.0003	-0.0020	0.0008	0	0
57	1400	-0.0024	0.0011	0.0013	0.0048	0	0
58	1422	0.0008	0.0002	-0.0010	0.0025	0	0
59	1435	0.0020	-0.0008	-0.0012	-0.0019	0	0
60	1454	-0.0003	0.0002	0.0002	-0.0002	0	0
61	1488	-0.0042	0.0022	0.0020	-0.0002	0	0
62	1495	-0.0002	0.0002	0	-0.0016	0	0
63	1533	-0.0021	0.0013	0.0008	-0.0004	0	0
64	1566	0.0013	-0.0006	-0.0008	0.0043	0	0
65	1566	0.0031	-0.0023	-0.0008	-0.0014	0	0
66	1583	-0.0015	0.0006	0.0009	0	0	0
67	3085	-0.0001	0	0	0	0	0
68	3090	0	0	0	0	0	0
69	3103	0	0	0	0	0	0
70	3106	0	0	0	0	0	0
71	3109	0.0001	0	-0.0001	0.0001	0	0
72	3111	0.0004	-0.0002	-0.0002	0	0	0
73	3119	0	0.0001	0	0.0004	0	0
74	3127	0	0	0	0	0	0
75	3132	0	0	-0.0001	0	0	0

8.8 Pentacene in *p*-terphenyl

i	freq.	Dxx	Dyy	Dzz	Dxy	Dxz	Dyz
1	38	0	0	0	0	0	0

2	55	0	0	0	0	0	-0.0001
3	60	0	0	0	0	0	0
4	80	0	0	0	0	-0.0002	0.0003
5	81	0	0	0	0	0.0002	-0.0003
6	90	0	0	0	0	0	0.0001
7	101	0	0	0	0	-0.0002	-0.0009
8	119	0	0	0	0	0	0
9	128	0	0	0	0	0	0
10	129	0	0	0	0	-0.0002	-0.0004
11	174	0	0	0	0	0.0001	0.0008
12	195	0	0	0	0	0	0
13	234	0.0001	-0.0001	0	0.0001	0	0.0001
14	250	0	0	0	0	0	0
15	265	-0.0003	0.0003	0	0.0001	0	0
16	301	0	0	0	0	-0.0002	0
17	336	0	0	0	0.0001	-0.0001	-0.0009
18	354	0	0	0	0	0	0
19	355	0	0	0	0	0	0
20	430	0	0	0	0	0	0
21	434	0	0	0	-0.0001	-0.0001	0
22	442	-0.0001	0.0001	0	-0.0004	0	0
23	461	0	0	0	0	0.0002	0
24	467	0	0	0	0	0	0
25	479	0	0	0	0	0	0
26	497	-0.0002	0.0002	0	-0.0007	0	0
27	534	0	0	0	0	0	0
28	547	0	0	0	-0.0001	0.0001	0.0003
29	580	0	0	0	0	0	0
30	598	-0.0001	0.0005	-0.0004	0.0001	0	0
31	610	-0.0002	-0.0001	0.0002	0	0	0
32	616	0	0	0	0	0	0
33	693	0	0	0	0	0	0
34	716	0.0002	-0.0001	0	0.0005	0	0.0001
35	724	0	0	0	0.0001	-0.0001	-0.0004
36	735	0	0	0	0	-0.0001	0
37	736	0	0	0	0	-0.0001	0.0001
38	746	-0.0001	-0.0004	0.0004	0	0	0
39	747	0	0	0	0	0	0
40	755	0	0	0	0	0	0
41	764	0	0	0	0	0.0001	0.0005
42	795	0.0006	-0.0003	-0.0003	-0.0001	0	-0.0001
43	802	0	0	0	0	-0.0001	-0.0007
44	819	0	0	0	0	0	0
45	824	0	0	0	0	0	0
46	831	0	0	0	0	0	0
47	850	0	0	0	0	0.0001	0.0006
48	861	0	0	0	0	-0.0001	-0.0001
49	877	0	0	0	0	0	0
50	881	0	0	0	0	0	0
51	884	0	0	0	0	0	0
52	891	0	0	0	0	-0.0001	-0.0011
53	897	0	0	0	0	0	0
54	913	-0.0001	0.0001	0	-0.0002	0	0
55	938	0	0	0	0	0.0002	0
56	938	0	0	0	0	0.0001	0
57	966	0	0	0	0	0	0
58	966	0	0	0	0	0	0
59	1035	0	0	0	0	0	0
60	1035	-0.0002	0.0002	0.0001	0	0	0
61	1109	0	0	0	0	0	0
62	1119	-0.0001	0	0	-0.0001	0	0
63	1149	0	0	0	0	0	0
64	1157	0.0002	0	-0.0002	-0.0001	0	0
65	1166	0.0001	-0.0001	0	0.0011	0	0
66	1180	0	0	0	0	0	0
67	1184	0	0	0	0	0	0
68	1195	-0.0019	0.0013	0.0006	0.0003	0	0

69	1218	0	0	0	0	0	0
70	1236	0.0003	-0.0003	0	0.0003	0	0
71	1263	0	0	0	0	0	0
72	1267	0	0	0	-0.0003	0	0
73	1269	-0.0009	0.0011	-0.0002	0.0002	0	0
74	1275	-0.0001	0	0.0001	-0.0007	0	0
75	1288	0	0	0	0	0	0
76	1318	0	0	0	0	0	0
77	1326	0	0	0	0	0	0
78	1367	0.0015	-0.0013	-0.0002	-0.0003	-0.0001	0
79	1380	-0.0001	0.0001	0	0	0	0
80	1394	-0.0001	0.0001	0.0001	-0.0003	0	0
81	1419	0.0011	0	-0.0010	-0.0002	0	0
82	1433	0	0	0	0	0	0
83	1438	0	0	0	0	0	0
84	1457	0	0	0	0	0	0
85	1463	0.0026	-0.0019	-0.0007	-0.0007	-0.0001	0
86	1479	-0.0001	0.0001	0	0	0	0
87	1494	-0.0007	0.0005	0.0001	-0.0024	0	-0.0001
88	1501	0.0025	-0.0018	-0.0007	-0.0005	0	0
89	1507	-0.0002	-0.0002	0.0004	0.0017	0	-0.0001
90	1540	0	0	0	0	0	0
91	1549	-0.0009	0.0006	0.0002	0.0003	0	0
92	1564	-0.0001	0.0001	0	0.0005	0	0
93	1581	0	0	0	0	0	0
94	1590	-0.0001	0.0001	0	0.0002	0	0.0001
95	3104	0	0	0	0	0	0
96	3104	0	0	0	0	0	0
97	3106	0	0	0	0	0	0
98	3107	0	0	0	0	0	0
99	3109	0.0001	-0.0001	0	0	0	0
100	3112	-0.0001	0.0001	0	0	0	0
101	3112	-0.0002	0.0001	0.0001	0	0	0
102	3115	-0.0003	0.0002	0.0002	0.0001	0	0
103	3129	0	0	0	0	0	0
104	3133	0	0	0	0	0	0
105	3140	0	0	0	0	0	0
106	3143	0	0	0	0	0	0
107	3156	0	0	0	0	0	0
108	3161	0	0	0	0	0	0

8.9 Pentacene in benzoic acid

i	freq.	Dxx	Dyy	Dzz	Dxy	Dxz	Dyz
1	25	0	0	0	0	0	0
2	53	0	0	0	0	0	0
3	55	0	0	0	0	0	0
4	77	0	0	0	0	-0.0004	-0.0001
5	78	0	0	0	0	0	0
6	91	0	0	0	0	0	0
7	100	0	0	0	0	0.0001	0.0010
8	116	0	0	0	0	0	0
9	123	0	0	0	0	-0.0001	0
10	125	0	0	0	0	0	0
11	172	0	0	0	0	-0.0002	-0.0009
12	194	0	0	0	0	0	0
13	233	0.0001	-0.0001	0	0.0001	0	0.0001
14	252	0	0	0	0	0	0
15	259	0.0003	-0.0003	0	-0.0001	0	0
16	305	0	0	0	0	-0.0002	0
17	337	0.0001	0	0	0	0.0002	0.0009
18	354	0	0	0	0	0	0
19	360	0	0	0	0	0	0
20	425	0	0	0	0	0	0

21	437	0	0	0	-0.0001	-0.0001	0
22	440	-0.0002	0.0001	0	-0.0004	0	0
23	463	0.0001	0	0	0.0001	-0.0002	0
24	470	0	0	0	0	0	0
25	475	0	0	0	0	0	0
26	496	-0.0003	0.0002	0	-0.0007	0	0
27	533	0	0	0	0	0	0
28	545	0	0	0	0	-0.0001	-0.0003
29	577	0	0	0	0	0	0
30	597	0.0001	-0.0005	0.0004	-0.0001	0	0
31	611	0.0001	0.0001	-0.0002	0	0	0
32	617	0	0	0	0	0	0
33	694	0	0	0	0	0	0
34	713	0.0002	-0.0002	0	0.0005	0	0
35	720	0.0002	-0.0001	-0.0001	-0.0001	0	0.0004
36	731	0	0	0	0	0	0
37	732	0	0	0	0	0.0001	0
38	745	0.0001	0.0004	-0.0004	0.0001	0	-0.0001
39	746	0	0	0	0	0	0
40	753	0	0	0	0	0	0
41	762	-0.0001	0.0001	0	0	-0.0001	-0.0005
42	791	-0.0005	0.0003	0.0002	0.0001	0.0001	0.0005
43	797	-0.0004	0.0002	0.0002	0.0001	-0.0001	-0.0006
44	807	0	0	0	0	0	0
45	823	0	0	0	0	0	0
46	826	0	0	0	0	0	0
47	845	0.0001	-0.0001	0	0	-0.0001	-0.0007
48	855	0	0	0	0	-0.0001	-0.0001
49	870	0	0	0	0	0	0
50	877	0	0	0	0	0	0
51	884	0	0	0	0	0	0
52	886	-0.0001	0.0001	0	0	0.0002	0.0010
53	895	0	0	0	0	0	0
54	911	-0.0001	0.0001	0	-0.0002	0	0
55	934	0	0	0	0	-0.0002	0.0001
56	934	0	0	0	0	0.0001	0
57	962	0	0	0	0	0	0
58	962	0	0	0	0	0	0
59	1031	-0.0001	0.0001	0	0	0	0
60	1031	0.0002	-0.0001	0	-0.0001	0	0
61	1102	0	0	0	0	0	0
62	1111	0	0	0	-0.0001	0	0
63	1138	0	0	0	0	0	0
64	1146	-0.0003	0.0001	0.0002	0.0001	0	0
65	1161	0.0001	-0.0001	0	0.0011	0	0
66	1173	0	0	0	0	0	0
67	1181	-0.0001	0.0001	0	0	0	0
68	1192	0.0019	-0.0013	-0.0006	-0.0004	0	0.0001
69	1210	0	0	0	0	0	0
70	1228	0.0003	-0.0003	0	0.0002	0	0
71	1259	0	0	0	-0.0001	0	0
72	1260	0.0003	-0.0003	0	0.0004	0	0
73	1261	-0.0007	0.0009	-0.0002	0.0003	0	-0.0001
74	1270	-0.0001	0	0	-0.0007	0	0
75	1281	0	0	0	0	0	0
76	1310	0	0	0	0	0	0
77	1317	0	0	0	0	0	0
78	1363	-0.0015	0.0013	0.0002	0.0004	0	-0.0001
79	1374	0	0	0	0	0	0
80	1385	-0.0002	0.0001	0	-0.0003	0	0
81	1413	-0.0012	0.0001	0.0011	0.0002	0	0
82	1428	0	0	0	0	0	0
83	1431	0	0	0	0	0	0
84	1449	0	0	0	0	0	0
85	1457	-0.0023	0.0017	0.0006	0.0009	0	-0.0001
86	1474	0	0	0	0	0	0
87	1486	-0.0012	0.0009	0.0003	-0.0021	0	0

88	1495	-0.0025	0.0018	0.0007	0.0010	0	0
89	1502	0.0007	-0.0005	-0.0003	0.0002	0	0
90	1537	0	0	0	0	0	0
91	1546	0.0008	-0.0005	-0.0002	-0.0004	0	0
92	1557	0.0005	-0.0006	0.0002	-0.0002	0	0
93	1573	0	0	0	0	0	0
94	1582	-0.0003	0.0003	0	-0.0001	0	0
95	3092	0	0	0	0	0	0
96	3093	0	0	0	0	0	0
97	3104	0	0	0	0	0	0
98	3105	0	0	0	0	0	0
99	3108	0	0.0001	0	0	0	0
100	3110	0.0001	-0.0001	0	0	0	0
101	3116	-0.0002	0.0001	0.0001	0.0001	0	0
102	3119	-0.0003	0.0002	0.0002	0.0001	0	0
103	3122	0	0	0	0	0	0
104	3123	0	0	0	0	0	0
105	3134	0	0	0	0	0	0
106	3135	0	0	0	0	0	0
107	3149	0	0	0	0	0	0
108	3149	0	0	0	0	0	0

9 Equilibrium Geometries at T₁ State

9.1 Naphthalene

C	2.47716500072648	0.68305138310426	0.00000078190402
C	-2.47716489636321	0.68305138988208	0.00000258012220
C	2.47716445858503	-0.68305186732199	0.00000012472389
C	-2.47716443353175	-0.68305188231256	-0.00000137630012
C	1.23566412211898	1.39635337234651	-0.00000083268509
C	-1.23566400144864	1.39635323105119	0.00000079407299
C	1.23566383730164	-1.39635293065928	0.00000101922610
C	-1.23566386402863	-1.39635279321056	-0.00000174756557
C	0.00000006093598	0.71910278074427	0.00000055352926
C	0.00000008660216	-0.71910193071680	0.00000074643400
H	3.41324062310589	1.23948412905279	-0.00000117974133
H	-3.41324051814101	1.23948410164417	0.00000165296745
H	3.41323997732272	-1.23948488479123	-0.00000429386668
H	-3.41323996801414	-1.23948492413858	-0.00000827747173
H	1.23755673716913	2.48671338687491	-0.00000177912429
H	-1.23755701050557	2.48671326239035	0.00000249983567
H	1.23755579178331	-2.48671298783704	0.00000471373607
H	-1.23755600361835	-2.48671283610249	0.00000402020313

9.2 Anthracene

C	3.69120268311073	0.69149735477405	0.00000034113708
C	3.69120215273474	-0.69149654730709	0.00000021341925
C	2.47192452312764	1.39343104554340	0.00000042610606
C	2.47192497683020	-1.39343154380927	-0.00000110995345
C	1.24661890272219	0.71775182788071	0.00000263003640
C	1.24661983371047	-0.71775182686174	0.00000182667217
C	-0.00000018067316	1.40122657287507	0.00000305814251
C	0.00000019481406	-1.40122665905425	0.00000303189620
C	-1.24661959381882	0.71775169425199	0.00000255943523
C	-1.24661942949663	-0.71775200755648	0.00000206461104
C	-2.47192483267992	1.39343140529830	0.00000132637287
C	-2.47192496703706	-1.39343140395514	-0.00000026112980
C	-3.69120276595658	0.69149739548450	-0.00000072044337
C	-3.69120268503501	-0.69149685097736	0.00000010910285
H	4.63116682906591	1.24169442371991	-0.00000057916097
H	4.63116582228373	-1.24169436319387	-0.00000125225586
H	2.47109196795939	2.48436800204884	0.00000095121463
H	2.47109137069048	-2.48436872047825	-0.00000110357123
H	-0.00000016171360	2.49315755345081	-0.00000811655974
H	0.00000097176492	-2.49315760008511	-0.00000258558424
H	-2.47109120436523	2.48436863171823	0.00000019305676
H	-2.47109134399674	-2.48436838128068	-0.00000205167779
H	-4.63116682021867	1.24169462347271	-0.00000150256436
H	-4.63116624382304	-1.24169462595931	0.00000055169775

9.3 Tetracene

C	4.90848964205431	0.69785247904259	0.00000329702089
C	4.90849120539274	-0.69785079456777	-0.00000074810264
C	3.70407326610312	1.39488519813090	0.00000816428804
C	3.70407624442788	-1.39488575952627	-0.00000678169122
C	2.47552635537278	0.71546542292190	0.00000409434140
C	2.47552804872646	-0.71546815372795	-0.00000010364848
C	1.22787636282213	1.40073813671619	0.00000606808744
C	1.22787863190794	-1.40074196268350	-0.00000115121756

C	-0.00000077045360	0.72648220092597	-0.00000144626974
C	0.00000105626598	-0.72648501903739	-0.00000069718143
C	-1.22787805459824	1.40073973428518	-0.000000610882219
C	-1.22787729157660	-1.40074010728201	0.00000112926766
C	-2.47552812503717	0.71546721309556	-0.00000203588248
C	-2.47552758774245	-0.71546628743385	0.00000389105707
C	-3.70407523483167	1.39488578327358	-0.00000584506112
C	-3.70407475687625	-1.39488392989098	0.00000772340327
C	-4.90849109670222	0.69785243913265	-0.00000331238107
C	-4.90849041195534	-0.69785003870888	0.00000066860785
H	5.85152076246390	1.24308786543073	0.00000669355222
H	5.85152397742131	-1.24308358465274	-0.00000791318786
H	3.70084859761541	2.48593936445196	0.00001071660088
H	3.70085478080138	-2.48594002145488	-0.00001144808780
H	1.23129921101733	2.49293170897378	0.00000374874096
H	1.23129805773186	-2.49293562655722	-0.00000868980769
H	-1.23129688714922	2.49293353258936	-0.00001030555483
H	-1.23129863082751	-2.49293368976503	0.00000269351333
H	-3.70085149108293	2.48594022427515	-0.00000855824411
H	-3.70085219051782	-2.48593804369924	0.00001331749960
H	-5.85152245676099	1.24308755490222	-0.00000560644254
H	-5.85152121401251	-1.24308583915997	0.00000854560217

9.4 Pentacene

C	1.23828610140037	0.72624384180274	0.00026813208043
C	1.23828563336537	-0.72622978780237	0.00027342694250
C	-1.23830366013326	0.72624225751299	0.00031629230327
C	-1.23830138776218	-0.72623138401871	0.00032350889996
C	-0.00000925750418	1.40388984273456	0.00028927835632
C	-0.00000748459873	-1.40387752532344	0.00029282164202
C	3.69875400596827	0.71554797614075	0.00024215192224
C	3.69875343232977	-0.71553720695171	0.00024813059849
C	-3.69877179867681	0.71554310741645	0.00037946723659
C	-3.69876909159087	-0.71554223496716	0.00038496275773
C	2.45657982110744	1.40016552025197	0.00025251853803
C	2.45657869679213	-1.40015228963420	0.00025790417172
C	-2.45659888576119	1.40016209828497	0.00035102316794
C	-2.45659353563650	-1.40015563247721	0.00035274088731
C	4.93329931770519	1.39729906223402	0.00022647499414
C	4.93329854743977	-1.39729021995004	0.00024641961477
C	-4.93331778640813	1.39729239652640	0.00040532477176
C	-4.93331328670823	-1.39729684451434	0.00042769523687
C	6.12813386402959	0.70239298990158	0.00022392459708
C	6.12813349430626	-0.70238497349620	0.00023607930803
C	-6.12815147305839	0.70238461224247	0.00044055901851
C	-6.12814952420912	-0.70239323566364	0.00045479383646
H	-0.00000989242800	2.49604859227096	0.00028837485359
H	-0.00000709976183	-2.49603642809067	0.00029319120276
H	2.45917361944007	2.49249556394057	0.00025038943705
H	2.45917148042044	-2.49248245602028	0.00026160848436
H	-2.45919414282961	2.49249215764047	0.00035332897806
H	-2.45918490087994	-2.49248579360715	0.00035759315092
H	4.92836621010825	2.48834830169051	0.00021748218301
H	4.92836438172976	-2.48833949709788	0.00025503641486
H	-4.92838628314385	2.48834165509814	0.00039477875862
H	-4.92837754525030	-2.48834611939862	0.00043692061524
H	7.07351828532259	1.24372878448870	0.00021407054403
H	7.07351711337208	-1.24372145724131	0.00023992086120
H	-7.07353652990489	1.24371929729440	0.00045544155766
H	-7.07353243859131	-1.24373097121775	0.00048623207649

9.5 DAT

C	4.83926579611888	0.69665661377069	-0.00000051303129
C	4.83926459859158	-0.69665903354243	-0.00000298352079
C	3.63278440230916	1.39597619006366	-0.00000356982410
C	3.63278266512222	-1.39597712579391	0.00000075160848
C	2.40625030804787	0.71592824081250	0.00000249179142
C	2.40624964329762	-0.71592755988591	0.00000459001765
C	1.16199237836431	1.40302064758377	0.00000174804482
C	1.16199130831670	-1.40301850365794	0.00000798613415
C	-0.07234086556816	0.72672384112093	0.00000154182216
C	-0.07234152946541	-0.72672035070782	0.00000311825175
N	-1.20828402376374	1.43518574148998	0.00000063700603
N	-1.20828264623961	-1.43518117367362	0.00000154307042
C	-2.37219258625796	0.71535821791811	-0.00000025853067
C	-2.37219062320941	-0.71535665046597	-0.00000143692564
C	-3.59870769966826	1.39968876835915	0.00000494321810
C	-3.59870453272427	-1.39968903027906	-0.00000636443882
C	-4.79723715808716	0.69993730588383	0.00000117396736
C	-4.79723531500271	-0.69993963875765	-0.00000231782278
H	5.78204263127877	1.24211921672840	-0.00000452919110
H	5.78204089190605	-1.24212283028650	-0.00000226401851
H	3.62962514786364	2.48672828376992	-0.00000556776839
H	3.62962094796670	-2.48672916477197	0.00000201868094
H	1.13780751124832	2.49394467568996	-0.00000361061919
H	1.13780411255985	-2.49394198282831	0.00000802619529
H	-3.56902002016901	2.48888507607295	0.00000523751926
H	-3.56901333640959	-2.48888506389776	-0.00000870435763
H	-5.74186979770417	1.24226229915160	0.00000364553817
H	-5.74186682012225	-1.24226700986660	-0.00000733281709

9.6 TrAT1

C	4.83533610890382	0.68112347675979	0.00000076283436
C	4.82456139522078	-0.71087658105168	-0.00000172207767
C	3.63305008101732	1.39089102935834	-0.00000034752067
C	3.61134302217103	-1.40124758358840	-0.00000120714708
C	2.40218399357220	0.72073706332599	0.00000040751787
C	2.39084212579992	-0.71131258080277	0.00000179951955
C	1.16366276791705	1.41781516059760	-0.00000085841096
C	1.14247916897901	-1.38884830555442	0.00000475329601
C	-0.07756534392802	0.74990502416409	-0.00000121745626
C	-0.09108687441157	-0.70212541555371	0.00000020700435
N	-1.20783834434603	1.46295361102129	-0.00000214000671
N	-1.22555761838281	-1.40695689075265	0.00000022656322
C	-2.37185679193267	0.74455399328572	-0.00000175823159
C	-2.38859179464288	-0.68824878388755	-0.00000135075913
C	-3.60101971054069	1.42015022825124	0.00000153103986
N	-3.53563570363348	-1.39281337823948	-0.00000412896379
C	-4.77020268406346	0.68129491545760	0.00000137990892
C	-4.68119301462075	-0.71706976722012	-0.00000336485575
H	5.78206158348462	1.21964702355777	0.00000022740147
H	5.76273356583346	-1.26409356905926	-0.00000405046074
H	3.63919112756429	2.48161295751188	-0.00000051605419
H	3.59965014684467	-2.49187966623311	-0.00000013236180
H	1.14804744957021	2.50891579904319	-0.00000092328450
H	1.10741774855512	-2.47939076223175	0.00000925070478
H	-3.59166353810399	2.50968987329960	0.00000308399688
H	-5.74576492526352	1.16476511341813	0.00000498559654
H	-5.59212698006364	-1.32026666877734	-0.00000489779297

9.7 TrAT2

C	4.84839039590527	0.68913224112289	0.00000706846286
C	4.84093943539510	-0.70412927710004	0.00000129296131
C	3.64546147130810	1.39381191640499	0.00000190331384
C	3.63136421941334	-1.39900819789777	-0.00000309190496
C	2.41581370594892	0.71813860943723	-0.00000178820929
C	2.40852221244595	-0.71361909097785	-0.00000167095917
C	1.17665225303887	1.41058195855438	-0.00000424160571
C	1.16117149095667	-1.39550883756924	-0.00000272146255
C	-0.06333486841271	0.73961235057063	-0.00000826751694
C	-0.06994334248463	-0.71503989057523	-0.00000505610228
N	-1.19174017014151	1.45946058039705	-0.00000891501249
N	-1.20977313178535	-1.41887102337712	-0.00000208408947
C	-2.35654578433205	0.73991713446788	-0.00000434855807
C	-2.36131939103652	-0.68503851774849	-0.00000195799043
C	-3.59643668563357	1.39210577039664	-0.00000027747210
C	-3.60625091742276	-1.34228581761645	0.00000414507008
C	-4.75861979214167	0.63258295500000	0.00000461770574
N	-4.77788963380192	-0.71294255064379	0.00000628070924
H	5.79386149430841	1.22965096470866	0.00001138140628
H	5.78108911037615	-1.25410545785148	0.00000186549564
H	3.64675395379347	2.48452052350911	0.00000405918594
H	3.62417912291596	-2.48964848132859	-0.00000391939238
H	1.15629396622586	2.50159644696484	-0.00000325394875
H	1.13241394575135	-2.48626431864720	-0.00000228875889
H	-3.62239178304052	2.48114550185329	-0.00000238367696
H	-3.61047856235047	-2.43511727114766	0.00000726498366
H	-5.73395118529974	1.12327222909333	0.00000638736587

9.8 Pentacene surrounded by nearest 16 *p*-terphenyl

C	7.699789088830962	-1.070729163873387	-0.855797908375143
H	7.508220079223923	-1.964491008516454	-1.445617618142515
H	7.752747402963760	-1.770558843559291	-3.408029332155440
C	8.402754771748889	0.010089034794150	-1.414126949717696
C	8.436102524648316	-0.986260746823456	-3.727474255068881
C	8.833906927046073	-0.964490549687665	-5.060446277062137
H	8.467601762513514	-1.736275778848582	-5.736626589409870
C	16.274056169680826	5.707038654866184	-1.476987014981274
C	7.596604127611767	4.654919002102408	-0.840967837079356
H	7.317297477553890	3.803181879072025	-1.457085892480094
C	16.292403207089752	4.738823991693767	-3.804500718886931
C	16.714263977954737	4.760088691672411	-5.130300494562700
H	7.797106832135763	3.861861079722790	-3.352488589891664
H	16.335670193421038	4.004673575856730	-5.817342688987669
C	8.614395225185278	1.115519236776672	-0.572700494838541
H	9.139941388770550	1.995843309267836	-0.937557919924185
C	8.366548919917221	5.701078106888710	-1.378139617375812
C	15.584367212612621	4.616501169822967	-0.921732773505278
C	8.867575404260787	-0.001150931273231	-2.820408706678268
H	15.396558010096831	3.725410612643963	-1.517076087114079
C	8.451529941246775	4.668194704685027	-3.677502320537954
C	9.732323184946384	0.993199737989398	-3.311559996249446
C	8.888952128118390	4.660487692506690	-4.997337301137598
H	15.582306815592313	3.971146972626376	-3.501980651370289
C	10.126414583698661	1.018279975273074	-4.645564868628934
H	10.114996111131010	1.764347289629240	-2.646786587829041
C	9.672749979896523	0.043970546214219	-5.532481018292845
H	8.566147394253406	3.855442019653432	-5.656610928785007
H	10.799057079208453	1.805978545953677	-4.982437165946781
H	9.968958172127522	0.071455910207972	-6.580158978985995
C	11.585534523544386	3.912188208675581	-1.034514301151047
C	12.371405339611528	2.875201543806813	-1.565851835161620
C	12.682386656145965	1.822990380668218	-0.688252817642113

C	12.828707892977905	2.876823277394258	-2.975133535251668
C	12.434247068779218	3.882508454967376	-3.876646967830268
C	12.834206035740767	3.856596910370916	-5.208409952987928
C	13.648438420135282	2.830487251945916	-5.685231725306362
C	14.063099575284497	1.833419346708001	-4.804992381961053
C	13.656053892216045	1.855319891137526	-3.475576658414976
H	11.302803488677689	4.761754836588324	-1.652003431772215
H	13.287853984615765	0.982607183710865	-1.020068878015543
H	11.787282473125968	4.695120442536890	-3.553316542207256
H	12.492928819287378	4.644800861518780	-5.878511029988324
H	13.954166741145716	2.807274171003876	-6.730266565274267
H	14.714186115012895	1.028455371672168	-5.142943543950803
H	13.996551500999393	1.053008029391975	-2.825962504891457
C	16.487338972803222	6.807148818221021	-0.628636689487749
H	17.001678682142774	7.694589789943647	-0.992445958816404
C	16.740402170624233	5.702566337022741	-2.882336502647238
C	17.639469192562835	6.676184643318385	-3.352273478450524
C	18.057844068323853	6.700501324707910	-4.678711187078335
H	18.034358994764133	7.429235588013649	-2.674324550301858
C	17.591978205213199	5.745422687008373	-5.580447242767487
H	18.760747407817966	7.469194207525702	-4.996789655907140
H	17.907333169700347	5.768406068193108	-6.623240091488828
C	8.675323980888122	6.754744980925129	-0.500348116119287
H	9.267210299541869	7.602824889277168	-0.837485621210583
C	8.827752262849327	5.691558675659756	-2.786636043937150
C	9.661765112671137	6.705984261552509	-3.290809292608795
C	10.101834445568217	6.697253870959142	-4.611172995218684
H	9.987378479227747	7.521563054163074	-2.649251649144137
C	9.717586026049524	5.674611127354407	-5.475181530369802
H	10.757809563568106	7.496158930891859	-4.954801155943894
H	10.053037168406552	5.672101187706193	-6.511396294296638
C	11.699322904857773	9.659360111237177	-0.947937361261776
C	12.358648723785640	8.547786171964873	-1.499488590469406
C	12.556272570342713	7.450162765134642	-0.643731685943527
C	12.815518785106891	8.534725313711828	-2.907954375806153
C	12.402266935629450	9.522820226005894	-3.820232116768690
C	12.818566943719496	9.499601090238542	-5.146832019757142
C	13.658357734949050	8.487312693027924	-5.608429685309762
C	14.085551176574594	7.504328655009308	-4.718462647098519
C	13.670755241647756	7.528601054696126	-3.390808058146625
H	11.528540530287282	10.551394346551927	-1.546652357907673
H	13.049537772145472	6.549482973585127	-1.003752342426669
H	11.726148844817224	10.315889683879767	-3.507574432583095
H	12.469198692669096	10.277012313818446	-5.825292895532950
H	13.974837045201646	8.463708306955670	-6.650396237811076
H	14.757405891308018	6.712428279657622	-5.046296378791340
H	14.033370266753877	6.749660462084810	-2.723898558343471
C	6.990306144582846	0.065165476466114	2.704149734752455
C	6.185071398689026	0.013295030537622	5.417228363734619
C	5.734023613583727	-0.961105603654024	4.529152334199678
C	6.129422410772937	-0.933570020675096	3.195311499127287
H	5.889685080937577	-0.018135362511335	6.465050816140897
H	5.062000711952555	-1.749854115313258	4.865381014084676
H	5.750914648768450	-1.707344947885779	2.531064548669544
C	7.240984864971175	-1.049635494236524	0.453640754626278
C	6.997260218978078	-1.004655081396918	12.765079499446745
H	6.715751877440613	-1.931002128006007	0.816253803549149
H	6.745147094136285	-1.872466663084346	12.158724468587391
H	7.054566790690842	-1.709632122834559	10.207835851482550
C	7.747993534712081	0.049596884027785	12.217478026629282
C	7.746196101286817	-0.930720487396037	9.891882116702188
C	8.146978037798666	-0.911723644045186	8.559438016547709
H	7.767117799409260	-1.675818667482404	7.881992263762587
C	6.410903628644570	0.084684780629679	16.365323098177022
C	5.588491087372103	0.063604888853570	19.076932358097125
C	5.120291732447041	-0.903391196510921	18.189356334938271
C	5.524461434432973	-0.890591202585123	16.857573507816941

H	5.282307712161535	0.049369246712648	20.122916718228112
H	4.429430506634192	-1.676675712950773	18.523718339479252
H	5.133234744554354	-1.659693527165771	16.195544443231942
C	6.567514715746508	-0.993039277592221	14.084988271774488
H	5.999449117902744	-1.852733532152486	14.434743268286423
C	-2.152720178777878	5.769623238260720	30.087763759939840
C	-2.988374679921472	5.719774560276011	32.793071110356074
C	-3.426380140412748	4.743263360337541	31.900552639585580
C	-3.016170954476896	4.770567636157693	30.571425062207716
H	-3.300535285779992	5.695650389416660	33.836951689322667
H	-4.102222596794727	3.954303202901928	32.227891874070785
H	-3.388551249472602	3.997300663189465	29.903724056761735
C	-1.910586003160944	4.672451944941042	27.828203732492955
H	-2.426985388241423	3.784974896646745	28.188595814897521
C	-1.694092830947978	5.770944942761675	28.678514430133674
C	-1.729597978955789	6.751871340284199	31.002623195855374
C	-2.142957329509853	6.727747723047317	32.331244848503459
H	-1.784351250722908	7.500260650118808	33.010305224806231
C	-1.465244430463381	4.665331229887528	26.514165212546409
H	-1.653053633014624	3.774240682708374	25.918821898978120
H	-1.467304827483691	4.019977032690933	23.933917334681404
C	7.454649600679309	0.055211935067058	1.296632056869102
C	6.264943835139108	11.519733873873786	28.602722403299154
C	7.024259233046427	5.720475742252933	2.766847554696998
C	5.794939279846628	5.826098658368401	30.027798511018119
C	7.415886697319614	1.052401839038776	3.612692527874678
C	6.226180941778739	12.516923777881400	30.918782874194147
C	7.019505887596686	1.026027356948870	4.946517243342797
C	5.829800132055810	12.490549295791492	32.252607589662261
C	6.158346176930231	5.723250709380084	5.462161765601014
C	4.929026223841152	5.828873625455429	32.723112731921447
C	5.713415550145892	4.741680577382352	4.579688109304563
C	4.484095596946092	4.847303493497820	31.840639065625684
C	6.140188916488096	4.741763136382913	3.255282609624222
C	4.910868963288297	4.847386052498379	30.516233565945345
H	7.382627045653336	1.798793865253259	5.623437417565038
H	6.192921290112460	13.263315804095878	32.929527763884508
H	5.832716543553426	5.720213804229675	6.501429991829391
H	4.603396590353626	5.825836720345139	33.762380948150508
H	5.016946095256881	3.972184774995860	4.910668745157974
H	3.787626142167805	4.077807691071203	32.171619711478399
H	5.762094231837331	3.963929270979675	2.596039377031142
H	4.532774278672986	4.069552177095288	29.856990333311746
C	7.170049242677181	4.659068589885300	0.479555144807279
C	5.940729289512832	4.764691496000911	27.740506101087881
H	6.583476839037232	3.808155910788107	0.819276137404636
H	5.354156885837432	3.913778826903574	28.080227093725760
C	3.113073576916199	3.926222647420686	12.767934122872278
C	2.952220495804093	1.850763884564587	28.184691678256868
C	3.749470764342798	2.804617365572818	12.207686578766529
C	2.253902972103045	2.946528186632115	28.719292607005396
C	2.023787695797148	4.026494737979069	27.848672183960350
C	3.953870619217576	1.711713189028425	13.068105477193070
C	4.174163383902412	2.772787385932023	10.789099164557774
C	1.790468908193806	2.960911525593970	30.125707163077060
C	3.842970704295703	3.812747156361351	9.901224439512699
C	2.213867037249901	1.984438465240666	31.046224635415413
C	4.226377390712907	3.775593648315796	8.565273725626632
C	1.794027856822948	2.011287264330691	32.371487544672320
C	4.952755816792374	2.694880683338511	8.067962351481246
C	0.939035781825877	3.015240174922799	32.823626799258797
C	5.296591782741378	1.657692153742931	8.932649470627087
C	0.499870021226790	3.984979159871114	31.925206360113084
C	4.915248247416354	1.696217493149628	10.269375759168634
C	0.919168583597679	3.957757634103130	30.598999355649809
H	2.931993534718070	4.815347720297661	12.167924590234220
H	3.153386181341096	0.973381484078751	28.795477263971740

H	1.498695997012570	4.914884613483094	28.194178687557816
H	4.440449723575588	0.806451472608753	12.711038160314903
H	3.259993109515434	4.665850314102397	10.240972908738810
H	2.901316945000445	1.197823923828688	30.742389975653595
H	3.942311693804230	4.598223377927677	7.909713624467418
H	2.152195990321660	1.244371626822868	33.057266706403396
H	5.250179837131039	2.665162911019945	7.020552783791174
H	0.622187322529339	3.044056505586362	33.865403877533382
H	5.881929343129041	0.810091281362035	8.579566093664944
H	-0.184585721312276	4.769114591364451	32.245132487433736
H	5.214558882038920	0.870179253091761	10.910997285474615
H	0.548381343643609	4.727689419186520	29.926367946382907
C	8.155058098343154	1.137459597989666	0.736731145142111
C	6.965352342837728	12.601981526832434	28.042821491421059
C	8.040717281866288	1.116868051166273	13.084573340769669
C	8.080331479525206	12.475767073893429	13.129712730768018
C	14.896891464333574	5.720793168196307	2.651865773847632
C	14.061236963189984	5.670944490211598	5.357173124263866
C	13.623231502698708	4.694433290273128	4.464654653493374
C	14.033440688634558	4.721737566093280	3.135527076115508
H	8.344960215439368	2.033299005952319	1.323958786771476
H	7.155254450009887	13.497820944718921	28.630049143200829
H	8.607398094500763	1.976744079277358	12.732621753640153
H	8.647012292124236	13.335643112004369	12.777761143679019
H	8.092135453859218	1.843747552899833	3.294746427677424
H	6.902429698318342	13.308269491742456	30.600836773996896
H	13.749076357185293	5.646820329392226	6.401053693271679
H	12.947389046281279	3.905473142837371	4.791993888019103
H	13.661060393603405	3.948470603124909	2.467826070710053
C	15.139025629915736	4.623621884840589	0.392305746551841
H	14.622626254870029	3.736144826582332	0.752697828805319
C	8.196933417574524	0.041563421839850	10.804847156869137
C	8.236547615233444	11.400462444567005	10.849986546867484
C	9.082523668834153	1.019072919671371	10.315950273967465
C	9.122137866457626	12.377971952398381	10.361089664006331
C	9.482009447327597	1.039664300548044	8.983222512945311
C	9.521623644986516	12.398563323275198	9.028361902943658
H	9.477105861652888	1.784113169097959	10.980721768390154
H	9.516720049312486	13.143012191789218	11.025861158499080
C	9.010271445957137	0.078265424767761	8.091889326711481
C	9.049885633616736	11.437164447459020	8.137028716820407
H	10.172122717464672	1.814161463085227	8.650775728059564
H	10.211736905088822	13.173060495776342	8.695915118209006
H	9.310308045787231	0.099705627008048	7.044592909460348
H	9.349922243410699	11.458604659735057	7.089732299499214
C	10.943597330886742	4.020929253344676	12.721629764981063
C	12.241009630831336	1.809891104272867	0.626205967969096
C	11.709595765476841	2.968632652682382	12.190523247160584
C	11.457041991188456	2.847030660802846	1.158915098507283
C	11.142004418397823	3.898202772828987	0.280606893860156
C	12.023762573632549	1.924929615532025	13.078638730920192
C	12.148192505487792	2.951233168575348	10.773676795740677
C	11.011385651045206	2.839992314725122	2.572066746862729
C	11.726542971635787	3.934203713451935	9.858684965689950
C	11.354766499259945	1.789766284626584	3.443214843275404
C	12.113101371537020	3.894473876625667	8.522698296536110
C	10.983098448685267	1.807774455200347	4.782530453867164
C	12.936459598157379	2.872489633640021	8.052921803415796
C	10.251186926134460	2.874154079442516	5.299620543107743
C	13.381113636326511	1.899362001549624	8.945829557757687
C	9.883072719692510	3.916039425616120	4.449414812489559
C	12.992083737064107	1.938366676873979	10.281036187799653
C	10.256776361283301	3.898504678595442	3.109931251622433
H	10.663126493085844	4.870369833789919	12.102047228481476
H	12.528381222353302	0.961495416917757	1.242615871480240
H	10.532647650074214	4.736258116236620	0.612603540800237
H	12.615691452905683	1.074183817100776	12.747646338335713

H	11.069475890099445	4.741395207593160	10.174949627932415
H	11.937758131670289	0.942543275492035	3.089767641357426
H	11.752468489780293	4.668908342238556	7.846797197085675
H	11.280844122113486	0.979632119187457	5.424499399382361
H	13.226661657454642	2.834868361885542	7.003345986379220
H	9.980092992522906	2.892605625952348	6.354212988319055
H	14.043344552055432	1.101248717701886	8.612689935312927
H	9.302201248896075	4.760925000334585	4.817960868566495
H	13.364313348076026	1.159883014794141	10.942846624328874
H	9.957448157317168	4.737289870560184	2.485359346275748
C	-1.005994126436999	6.862797977298156	28.122001987060152
C	16.043617516674455	6.813967907233743	0.686104000967948
C	7.478756113743096	5.712866225366810	1.356902074884193
C	6.249436160543300	5.818489141482277	28.617853031205318
C	5.800600389041970	11.529687415308734	30.010240081071931
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H	11.441655720720448	6.824189568295516	16.912707575784637
H	10.742679766851435	6.894582480190095	19.239981832443597
H	9.412009405612675	8.818386863041255	20.114619435029631
H	8.768909506436298	10.660814460340269	18.545218425554772
H	9.453479054438233	10.598427638198650	16.218954929688859
C	7.335245388966483	5.044851968565021	12.455874136929978
C	8.000001974531813	6.330690279983481	12.584378481612985
C	6.606755456734436	5.168674851280523	14.812411407565893
C	7.271580399181566	6.454375870173124	14.941133649656303
C	6.658815348807018	4.505609809917301	13.570216346861921
C	7.949560915806282	6.992702929887547	13.827046178849677
C	8.016724198078562	4.947808352900225	10.101310307187262
C	8.676574113515612	6.217573353377283	10.224245132128033
C	5.926091490597360	5.285597808954044	17.173067618938607
C	6.586753498088898	6.555449230648073	17.296293409292609
C	7.377084726963954	4.384931040333679	11.230114113235828
C	8.657806715138319	6.874081855942462	11.479041264591901
C	5.948150806186655	4.627224476764420	15.918669463679000
C	7.232152961904945	7.112874027838159	16.167750139575876
C	7.982878900026388	4.311511738710111	8.847190846447127
C	9.290749105353921	6.778675977448809	9.084463507805699
C	5.308388622013229	4.727057035918012	18.312777597869921
C	6.613693376556554	7.197222311211566	18.548175104887093
C	8.554916207638723	4.907123362477583	7.738949208191197
C	9.219270703840055	6.136523027238975	7.858593973849820
C	5.371305702175582	5.375173887195631	19.536570327753800
C	6.032715588469395	6.606228961576229	19.653960671825189
H	6.156583095538683	3.544504297888364	13.463127015530823
H	8.453891925802608	7.952994333325370	13.929632974029250
H	6.876960414626700	3.422778028077269	11.121316311395795
H	9.154856840055324	7.839564064827334	11.577397507452574
H	5.453990467937654	3.660365960510080	15.819916295379777
H	7.738067422665927	8.071752186461005	16.275541543352858
H	7.479587378823468	3.351426331757291	8.762668291217896
H	9.807968116743178	7.733474791947885	9.179122219143977
H	4.791847929705375	3.771526118071563	18.219655855355036
H	7.119359589154148	8.156709464563155	18.632940333937643
H	8.470665003238873	4.426876026865056	6.768550988750620
H	9.671829657902034	6.586880577463868	6.978527669544646
H	4.920857960913785	4.927634103341391	20.418842785248156
H	6.109003521616528	7.090526961158195	20.622360934625210

9.9 Pentacene surrounded by nearest 14 benzoic acid dimer

H	-1.550131596092891	-0.108934330946573	-4.805312202241158
H	3.921447281154851	-0.141816426994407	-4.784571155395215
O	-1.126760182930124	3.835633840174201	-0.166528058765792
C	-0.383844709713985	3.637137171956927	-1.152110629618296
C	-0.697130391221679	2.602162454846026	-2.163051619257741
C	-1.856902938638541	1.828976615816198	-2.025372055626264
C	-2.158007929294032	0.856783882453260	-2.975216051494737
C	-1.308583875565380	0.652373081992846	-4.063280225059305
C	-0.150275586798797	1.418768450834865	-4.198304909720690
C	0.155443582246912	2.389975535517766	-3.253831199797514
H	-2.514091799675661	1.988000512269733	-1.171666575296301
H	-3.054662450326776	0.250462657287351	-2.855738162321027
H	-1.610860137761238	4.938645732372525	-4.792197690937018
H	0.522424654127825	1.254504579976834	-5.039580718803700
O	-1.107734933063053	8.874124905312225	-0.158464445253083

C	-0.377964762560492	8.682436110856479	-1.155155656490512
C	-0.705693472350650	7.647865845572057	-2.161991377809851
C	-1.862846184761706	6.874563424939033	-2.003851794730791
C	-2.183526661658188	5.903846851908471	-2.948638714106854
C	-1.355876040089258	5.699676995752831	-4.053681740225299
C	-0.200225271452090	6.467044874634492	-4.208064283468808
C	0.126029138369052	7.437140648942425	-3.268533915924436
H	-2.503688148422222	7.034574558245692	-1.138108408127046
H	-3.079651992207220	5.300106872209559	-2.814386284970666
H	0.455176249130016	6.303818252873768	-5.062195083089966
O	4.370780583003130	3.847908887968481	-0.195431520174845
O	0.721228540326881	4.318890426099141	-1.374366465478680
C	5.115511829574030	3.638840110046091	-1.177885240115515
C	4.794336568474765	2.599667302643684	-2.181876797240523
C	3.640395867610715	1.822167066273074	-2.021084369480354
C	3.330660659670389	0.839515698217578	-2.956844867416159
C	4.165222460048331	0.630538705649618	-4.054921152216016
C	5.314113044307132	1.405851693666222	-4.217266022337167
C	5.630652068950212	2.386170540939522	-3.285247064850861
H	2.992474817046057	1.988310449248151	-1.161839007389540
H	2.437837053888791	0.231821303778172	-2.820746461911416
H	3.957002955237073	5.004721814838141	-4.857026855994066
H	5.969453746450288	1.236899212153701	-5.070355281324959
H	1.063339681350327	2.982331564858540	-3.342125016865698
H	0.873378982093027	5.056510356952463	-0.653214810714561
O	6.226445998008950	4.310569537219353	-1.398549079702764
H	6.530221362845208	2.988212138521381	-3.394889818830107
H	6.385338466660992	5.047680808216787	-0.678028346422424
O	4.440723332826700	8.892176487150543	-0.181489412332080
O	0.719208590400816	9.370967017479403	-1.391878712814453
C	5.179915171116890	8.701346769679072	-1.170989861259438
C	4.856705918426292	7.676779313907492	-2.190581975399029
C	3.691573665585743	6.912194924600590	-2.052639774535320
C	3.374844448007163	5.952881890348917	-3.010053705473188
C	4.212281987240419	5.755935793161146	-4.109270227673930
C	5.376613738826095	6.513622718173530	-4.245675760337377
C	5.700733318930321	7.467084828447391	-3.288330613925236
H	3.042339370403384	7.070560488079678	-1.192754012833575
H	2.472475329926754	5.355118806613006	-2.889961023087748
H	6.040702240548006	6.351139241880504	-5.094001115840822
H	1.030495193358647	8.032220129935025	-3.374935388737104
H	0.875600697258752	10.108764234302672	-0.670441564768188
O	6.284836897598539	9.383099803793060	-1.391081246283445
H	6.618253646305069	8.045334463092313	-3.370597928602015
H	6.437622544411679	10.116390571954671	-0.663944944402116
C	11.385324590686874	-0.618268386231308	12.965967173944552
C	11.662244156367883	-1.564284831456162	13.948304747358755
C	10.784306110451348	-1.741618489838397	15.018481801351612
C	9.623921727094940	-0.970626665630701	15.104670221065984
C	9.339962890267092	-0.027421903920942	14.125468339561266
H	12.061141565794550	-0.478175574760129	12.123560796685959
H	12.563306118397815	-2.170033517662334	13.867822442579584
H	0.843273006238207	-0.051470667955479	16.869739260835807
H	11.004975733089035	-2.486027381972314	15.784174575942790
H	8.931216974268967	-1.114441948553158	15.932485589181042
C	5.818169667014172	-0.592077063295767	12.978513156560407
C	6.110599579051280	-1.550578784212388	13.944360757295371
C	5.249656721584410	-1.741637606912863	15.025705942160936
C	4.089244558246103	-0.974809958646659	15.138589152498815
C	3.792057382775074	-0.018622541776851	14.176393665714325
H	6.482489131226314	-0.438715757623588	12.129298070695855
H	7.009557911599604	-2.155917577887302	13.842861619082390
H	6.448627734337096	-0.006505976406788	16.826600170112581
H	5.483361427713973	-2.494329239657117	15.778839301702735
H	3.408634650189996	-1.129604809874267	15.974538143365194
C	-3.360364959345045	15.837811328065428	8.742542853426027
C	-3.632308035837512	16.781642651797338	7.757130438186540

C	-2.751877843321910	16.952426231609053	6.687940155242090
C	-1.593947834710829	16.177352200316811	6.605964772293672
C	-1.314076536080347	15.237363040458545	7.588687915903249
H	-4.038570126977675	15.700813356665464	9.583633521189238
H	-4.531202253271075	17.390960679801111	7.835086708209849
H	-2.968412029965479	17.694726664092002	5.919361777142928
H	-0.899789693582423	16.315024940155240	5.778947740970756
O	-0.692967688758791	5.703025745562396	1.517888876037844
O	-0.674406382608749	10.736792556313487	1.518135798141010
H	-1.044564074293219	7.078458911711358	3.465165150388825
H	-1.024839331017332	12.096935936810505	3.468555521598613
H	-0.842434489283353	4.959807283490369	0.801874297024643
H	-0.824733072417224	9.993922887758160	0.801494843294771
O	-2.659351408975279	8.811126985689434	10.679565153724811
O	-2.713021466800041	13.875936361810570	10.658100042171514
O	-2.199041274717254	6.997715006509241	12.392656597231433
O	-2.378916036026352	12.066292406732924	12.391240424983756
C	-1.956010004235065	8.960318109111231	9.655342808193861
C	-1.916219733422877	14.063335847130368	9.712763039205226
C	-2.257221915092711	10.007127950575402	8.657097001898977
C	-2.197108987418774	15.062892463518004	8.660922811302409
C	-3.335691503131990	10.876662092268417	8.866827989456723
C	-3.620091030988079	11.863203038920926	7.928021322161628
C	-2.829172104294183	11.992060956385046	6.785424137997980
C	-1.750028591558551	11.131732633625466	6.579058318392963
C	-1.465451065724302	10.140914324290533	7.509562380508157
H	-3.942545891980282	10.778860483807351	9.765872734410660
H	-4.457933612368291	12.537014298025861	8.098766790084406
H	-3.053509017225916	12.768596176217233	6.054726922533624
H	-1.121092655219317	11.240366064707615	5.696785969208710
H	-2.495941897750998	5.718332967259230	14.396728562346540
H	-2.969233334797551	10.539865438533379	14.167821807192293
H	-2.354880613637180	7.732900036061855	11.666681858260143
H	-2.492695616973614	12.792505553265993	11.644826185121019
H	1.630357400727648	15.143067563408493	4.953687083720006
H	9.629116731157634	15.245495917948276	26.585599456073748
O	2.783893553429797	3.651597977767769	10.504911949821242
O	1.292606318066194	3.938254647061570	21.458878886036068
O	10.728220700683586	1.347283100131747	11.053935438232834
O	10.377032225919596	3.158365806493803	9.313441317023644
O	8.719987870777135	4.421318780595676	20.257545916874946
O	3.239627594875670	1.874661155470911	12.258697918178923
C	3.567582783575112	3.874822266070176	9.559109360462326
C	2.037337564637093	3.729185869139179	20.476425166095400
C	9.935001786183829	1.155286908719071	12.001060439273557
C	3.280571851705192	4.915035159276459	8.546232593625295
C	1.716162303537830	2.690013061736768	19.472433608970391
C	10.220585121063952	0.154071262888636	13.051856596246701
C	2.188280004721372	15.808964256960081	8.737797118426064
C	0.562221592673805	1.912512825355251	19.633226036750781
C	0.232727031359481	4.335447063475128	12.903346250280556
C	11.309660626726405	4.347529658921825	12.880948216423381
C	1.911729303541908	16.768508371267668	7.768159269847134
C	0.252486384753748	0.929861457256504	18.697465548814865
C	0.526923514792834	3.354519478276793	13.845047372687555
C	11.603857110159755	3.366602073723492	13.822649338830377
C	2.783125418749516	16.951696814267741	6.693918430389316
C	1.087048185111422	0.720884464731797	17.599389254015119
C	-0.259946149220168	3.223663946506251	14.990257280121758
C	10.816987446146754	3.235746541952950	14.967859246264581
C	3.938681653790564	16.176052932766446	6.592532482424753
C	2.235938779390463	1.496197452716057	17.437044393873634
C	-1.347751989083358	4.073993809115530	15.193086842020314
C	9.729181606283563	4.086076404562228	15.170688808163137
C	4.221020161397231	15.220403257356629	7.559677375764769
C	2.552477804033544	2.476516299989359	18.369063351359944
C	-1.642610725124994	5.058689057543180	14.259119925301574

C	9.434322870241926	5.070771652989878	14.236721891444397
H	1.515457596980402	15.661451860774434	9.581116576978099
H	-0.085699457870585	2.078656208287078	20.492471408841478
H	0.837554499747485	4.434635881611155	12.003400452806311
H	11.914488095114407	4.446718477057853	11.981002418949135
H	1.015588284258203	17.379666913713354	7.859803956280821
H	-0.640337211048144	0.322167062871259	18.833563944299499
H	1.370322114744151	2.687662038683944	13.675691115492544
H	12.447255710111072	2.699744634130643	13.653293081635368
H	2.560034502620785	17.703529051375117	5.936732016338331
H	0.878828690320404	5.095067573887979	16.797283560216737
H	-0.025423387351279	2.453111309064535	15.724885071223458
H	11.051510218015615	2.465193904522140	15.702487037346062
H	4.626519337477072	16.323129570615801	5.761181643707491
H	2.891279481513352	1.327244971246790	16.583955124885957
H	-1.973438905523734	3.963565079267556	16.077373514551887
H	9.103494689843188	3.975647674714254	16.054975480694708
H	10.950682216494588	4.687895004441181	7.533071509092644
H	9.062099011800580	3.084759919355076	18.289787365487928
H	2.883953639028860	0.575237525357251	14.246470095013954
H	10.496548603795382	2.434936443743169	10.058741977148891
H	8.872138312523012	5.158938711492246	20.978697561639176
H	3.082029098569794	2.589305982459377	11.513229125217482
H	7.180841288706761	15.199597125405594	4.908866271001004
H	4.102667023769824	15.289942884498679	26.563176677211921
O	8.439016492412723	3.629170641648942	10.380542542937228
O	6.871999147499861	3.938062194713984	21.465384313587947
O	5.109824997357887	1.385818627324194	11.086624701269139
O	4.698395065755273	3.222018445749970	9.378642116771010
O	3.148271723072042	4.400915296301529	20.255761326528365
O	8.802620046008263	1.811545047319654	12.143137725963449
C	9.245534614415039	3.814857133550587	9.444178901013606
C	7.614914620736268	3.739565526453463	20.479801752735327
C	4.352075812643936	1.199151148385927	12.063812774242123
C	8.980700172311611	4.816953188425291	8.386403819670146
C	7.301628939208307	2.704590809385813	19.468860753095996
C	4.656001636015445	0.179732362940779	13.092737107209524
C	6.141856391791446	1.931404970355981	19.606540316727475
C	5.840751401135954	0.959212236993042	18.656696320859002
C	6.690175454864606	0.754801436532633	17.568632147294434
C	7.848483743651459	1.521196805331398	17.433607472632929
C	8.154202912676897	2.492403890057549	18.378081172556225
H	5.484667530754324	2.090428866809517	20.460245797057432
H	4.944096870103236	0.352891011816229	18.776174210052933
H	6.387899192668748	5.041074086912307	16.839714681416723
H	8.521183984557810	1.356932934516617	16.592331653550040
H	4.979723908474115	4.424636590630096	7.323664964818164
H	3.452047097928541	3.078557897571216	18.259420597380693
H	8.429270680170708	0.565556555096919	14.169837448782559
H	4.837738120960583	2.482496784583724	10.103592881639546
H	3.307164201734876	5.138026557309971	20.976282059745216
H	8.675630649733144	2.523012990316539	11.395494861478092
O	1.159566432114255	6.174725183412488	0.312532740310036
O	9.158325762544241	6.277153537952271	21.944445112663779
O	1.166406825659541	11.222953912283185	0.300620237142345
O	9.165166156109798	11.325382266779718	21.932532619495966
O	4.818191558184102	5.704557290654211	1.482059828582203
O	1.740017283267460	5.794903049693138	23.136370244813229
O	4.880918952690028	10.735869453686472	1.527065711756093
O	1.802744687773361	10.826215212736306	23.181376127966892
C	0.413632452908734	6.381649814000277	1.293577848306432
C	8.412391783338721	6.484078168540064	22.925490220660166
C	0.427985969682811	11.420181555876564	1.289957012840958
C	8.426745300112799	11.522609910416350	22.921869385194697
C	0.728884992018970	7.424534149296351	2.296531899865458
C	8.727644322469223	7.526962503792884	23.928444282219083
C	0.746409032549214	12.453950142420705	2.299672589829363

C	8.745168362979200	12.556378496960491	23.931584962183106
C	1.898335912927725	8.183177338704912	2.159725233285641
C	9.897095243357711	8.285605693244694	23.791637605639380
C	1.916151591218774	13.212214860448761	2.166873840994288
C	9.914910921648762	13.314643214988548	23.798786213348027
C	2.205133562636127	9.161594996619524	3.101371601100061
C	10.203892893066111	9.264023351159310	24.733283973453794
C	2.228088697796069	14.176912972711950	3.120576472568079
C	10.226848028246323	14.279341327208481	24.752488854921701
C	1.350986999311505	9.389730874205982	4.181296384757021
C	9.349746329741492	9.492159228745768	25.813208757110758
C	1.378650321870782	14.389712541308423	4.206992898031089
C	9.377409652300770	14.492140895848205	25.838905270384828
C	0.182051482810282	8.638906107491643	4.312841661637665
C	8.180810813260535	8.741334461988176	25.944754043991288
C	0.207621978239600	13.641133006159926	4.334234328121512
C	8.206381308669588	13.743561360699712	25.966146700475246
C	-0.129813312300814	7.660444432242760	3.376966679053496
C	7.868946018129170	7.762872786782543	25.008879051407234
C	-0.108242254200701	12.676719316705981	3.386434033264634
C	7.890517076249553	12.779147671202514	25.018346415618254
H	2.559749980947398	8.004647785533832	1.313244809451716
H	10.558509311397650	8.107076140030363	22.945157191805343
H	2.573656011219878	13.044807424646578	1.315182905036695
H	10.572415341649865	13.147235779186360	22.947095277390439
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H	11.110227190374303	9.855660213986708	24.615761157921249
H	3.134259273637095	14.769836938498269	3.006680156980660
H	11.133018604067084	14.872265293038051	24.638592529334403
H	1.595418520470594	10.157153431635246	4.916900852092799
H	9.594177840900606	10.259581786164121	26.548813224466763
H	-0.495146383993800	8.821760384424254	5.145761614961663
H	7.503612946436187	8.924188738964041	26.777673987315403
H	-0.466739237353508	13.814315786300305	5.172245280864983
H	7.532020093076481	13.916744140840089	26.804157653218716
H	4.495118855509080	7.018282030693923	3.463211288584537
H	1.416944590572144	7.108627789787012	25.117521694795450
H	4.580703361595821	12.054924262348781	3.535573351144410
H	1.502529096658886	12.145270021441865	25.189883757355322
H	4.662521346102446	4.963600317208180	0.762366591297786
H	1.584347081165512	5.053946076301265	22.416676997508702
H	4.726738151065115	10.003134582525337	0.801831073449936
H	1.648563886128179	10.093480341618426	22.456141479660847
O	2.865483780970054	13.820972275366859	10.635736840404711
O	1.362549067910030	8.982522246200377	21.472821003878721
O	-0.448009505514395	6.399387196192731	11.093867735309932
O	10.628924089852529	6.411469791639430	11.071469701452754
O	-0.435191743444101	11.587872168422338	11.337876449177752
O	-0.907797875408964	8.211590063817365	9.382350992843577
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O	-0.786064839786430	13.403859368720152	9.573795891811931
O	8.717967920851070	9.473395371975940	20.240033669539169
O	3.264708810172158	11.990542254825080	12.357410281748766
C	3.6371110987412380	14.011860926153854	9.670724355901836
C	2.101740906179955	8.791692528772160	20.483320544951475
C	-1.152984512403072	6.247374769282443	12.116742294129697
C	9.923949082963851	6.259457364729140	12.094344260272520
C	-1.248941802179617	11.406991912769877	12.269212948106331
C	3.346224803411241	15.029341099639408	8.635835912424367
C	1.778531653489356	7.767125073000577	19.463728430811891
C	-0.852030637501179	5.197483499012240	13.111498326319028
C	10.224902967865717	5.209566094469846	13.089100292441632
C	-0.992666352583350	10.407391827507208	13.331010037299990
C	2.172822075250042	5.753334617533458	8.707981536197302
C	0.613399390648834	7.002540683682767	19.601670631695814
C	0.263422221569787	9.797153430334902	13.416972627275655
C	1.914437064561148	6.750749006324709	7.771810382323560

C	0.296670173070254	6.043227649431094	18.644256700757950
C	0.504405323806282	8.841820805410293	14.398617553815821
C	2.745978038407331	6.906063766204927	6.663885500052274
C	1.134107712323777	5.846281552200076	17.545040188557088
C	-0.50199998237470	8.492501852518220	15.300584957094266
C	3.845180255000322	6.062607674666381	6.495523383115147
C	2.298439473909427	6.603968477223365	17.408634655873424
C	-1.749104254111746	9.109973593722531	15.222992438164241
C	4.116424581202192	5.076460002430143	7.434687137546399
C	2.622559054013654	7.557430587497226	18.365979802285565
C	-1.993931890368903	10.065861677724579	14.244958727054325
H	1.529968178897166	5.629194187756372	9.577614111030901
H	-0.035834894513284	7.160906247129516	20.461556403377227
H	1.045461042989626	10.096219457406979	12.720944209725689
H	1.065481593111856	7.415425419226568	7.918542990769776
H	-0.605698935010182	5.445464565706095	18.764349383123168
H	1.485699667062049	8.374598313822332	14.468242211141371
H	2.539208619373213	7.687985196273820	5.933387457678664
H	-0.304450930651197	7.743359056809556	16.067495460599289
H	4.497915621544118	6.179851960181539	5.632261557781185
H	2.962527975611072	6.441485000973592	16.560309290370089
H	-2.539169611010395	8.841987543652596	15.921996719145751
H	-0.618466899066255	9.473517242103947	7.370753830793635
H	10.458466696300665	9.48559837550645	7.348355796936458
H	-0.405596925127855	14.640716944646213	7.547017119182631
H	9.029254523808900	8.134648484431560	18.256976993616522
H	2.982918218684405	10.794902968265980	14.427226372576124
H	-0.750736580786779	7.477350883406394	10.109470219111595
H	10.326197014580142	7.489433478853092	10.087072185254417
H	-0.663354111513503	12.693217936029560	10.323305604009880
H	8.874360027688738	10.211192588842456	20.961470807585549
H	3.128500632267535	12.725649011172747	11.627184298541481
O	6.684549684526257	6.162079975229373	0.293125337672931
O	3.606375419609591	6.252425734279211	21.947435753883731
O	6.724346364912813	11.220408024980014	0.314152906364271
O	3.646172099975877	11.310753784073098	21.968463312575182
O	7.305791641671195	5.805454100102179	23.149801248391579
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C	5.935309431707548	6.368789191248109	1.271856018543236
C	2.857135156770640	6.459134950330290	22.926166424774372
C	5.986627636113113	11.415681660418372	1.304233446377225
C	2.908453371176176	11.506027419511460	22.958543852588139
C	6.256601800872470	7.396380556422404	2.288787435848592
C	3.178427535935535	7.486726315515488	23.943097842059508
C	6.310075706439836	12.448857466576648	2.314254458686520
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C	7.418870409894421	8.165592344629287	2.152809214876923
C	4.340696144957485	8.255938103722375	23.807119621087836
C	7.463190680728060	13.226797849147765	2.152025711718599
C	4.385016415811393	13.317143608197600	23.806336127929399
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C	4.642844786814039	9.226462277456822	24.758466262320756
C	7.772634328117749	14.212370515796286	3.084683759883518
C	4.694460053180840	14.302716274878467	24.738994166114651
C	6.874183220405850	9.337532075614842	4.195176643238646
C	3.796008955468913	9.427877834707926	25.849487049449561
C	6.937199119750719	14.424976220629594	4.181396303582383
C	3.859024854813785	14.515321979722678	25.835706709793300
C	5.716639964099757	8.570039637180813	4.332987514303714
C	2.638465689183116	8.660385396219739	25.987297930534737
C	5.792411443103068	13.644662789310921	4.348855999468045
C	2.714237178166134	13.735008548404011	26.003166405678954
C	5.406309867952212	7.606478795761308	3.381424658879356
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C	5.477701713860540	12.659703096750992	3.421010260292357
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H	4.999049306128284	8.095158977827316	22.954533052371957
H	8.108563299311243	13.060145684833428	1.291153165575134
H	5.030389034394575	13.150491443883265	22.945463581785937
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H	8.665275699834851	14.819725993830797	2.946333532209874
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H	4.038730513293440	10.190694827545505	26.589659925342026
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H	1.968540990612516	8.823356722868811	26.830955071194239
H	5.139311836704066	13.811759367120052	5.203955822439768
H	2.061137571767132	13.902105126213137	26.858266228650677
H	6.954195256136767	7.180887266251141	25.097077522742559
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O	4.755987860109508	13.342200368554696	9.493207069921288
O	3.206662632661605	9.473445562886148	20.263229159927473
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C	8.819711680274208	10.019210546022100	8.634698968041800
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C	7.456842574378816	11.875285634378532	7.905623288284231
C	5.815232668771797	6.006275206448254	18.683273658246883
C	6.052830315564494	8.472434577251937	13.988104334338573
C	8.475596797325895	6.738237860811537	6.424985380218270
C	8.247761491072740	12.004143551831746	6.763026104140804
C	6.642883290340728	5.802105350292617	17.578230632128438
C	5.223599838621976	8.322611321394918	15.098744725729638
C	9.722949224389968	6.119989273362068	6.492020805864768
C	9.326905013808346	11.143815229083071	6.556660284515567
C	7.798534058998163	6.569473229131028	17.423848098884818
C	4.122787953017771	9.164698961783090	15.263789668613629
C	9.974779094914375	5.161752215081079	7.465817977576656
C	9.611482529642618	10.152996919737230	7.487164346650981
C	8.124788468799039	7.539569003482208	18.363378456429299
C	3.847424338443162	10.144268271237930	14.318185337820941
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H	7.134387703386641	10.790943079254049	9.743474700553483
H	5.495071182007764	7.137002912785475	20.493803964226693
H	6.431432036127646	9.584621308246124	12.174680472660937
H	6.494322496638336	6.854416345076070	7.273141873118310
H	6.61899982998630	12.549096893472559	8.076368756227229
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H	6.902219917083535	7.807759053846521	13.842538813184570
H	8.271531982688366	7.487523005787475	5.660021140287123
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H	10.506706330692413	6.387112487996065	5.785640244122434
H	9.955840940147606	11.252448660154313	5.674387935351533
H	8.453935579560001	6.406246607413554	16.569717289263771
H	3.472885225622258	9.051718394979259	16.129960676824076
H	5.126681421338941	14.621813782369184	7.499666966733116
H	3.540079381368132	8.135680222185398	18.283712477608901
H	8.580991697615923	5.730415562705929	14.374330528489363

H	4. 901576813552422	12. 624501341261574	10. 237512360295559
H	3. 359448269474771	10. 206736331036849	20. 990365461829022
H	8. 722052981729741	7. 744982631508553	11. 644283824402965
C	3. 626329714437208	6. 782208804536155	12. 042798358414707
C	4. 905147310512449	6. 568416323565785	11. 387226504212290
C	3. 102531923561310	8. 579226062238526	10. 418200729504351
C	4. 383112503543516	8. 368528764066038	9. 764941115327620
C	2. 763304241823540	7. 769895116378839	11. 525364554249643
C	5. 244556369171173	7. 378605609379508	10. 280731661839898
C	4. 181857409261527	5. 034823186054439	13. 689051224445064
C	5. 428853230567798	4. 800357667595236	13. 015259805307402
C	2. 575534556603765	10. 343254589527859	8. 787079343658590
C	3. 827146083666491	10. 116825043837103	8. 119444635742346
C	3. 304846011064817	6. 017904992050009	13. 166458662611786
C	5. 755601454262147	5. 577932559665525	11. 876922391696580
C	2. 250146623173008	9. 566158615062268	9. 925737755312392
C	4. 707648201086111	9. 138248638797139	8. 645293535939286
C	3. 884907523278271	4. 279631908485924	14. 844062314628502
C	6. 300507086984227	3. 811171952726123	13. 513492928023222
C	1. 697117146683095	11. 323466556673273	8. 283789889492608
C	4. 123027473374363	10. 874206721338494	6. 965860720943413
C	4. 777586544320855	3. 335571870561468	15. 327316283859535
C	5. 983874322802546	3. 093435110857740	14. 654280009507863
C	2. 013452285201101	12. 045138445013723	7. 145424828035321
C	3. 225884269606360	11. 812849877568535	6. 479451715278409
H	1. 787536123422274	7. 904597314635798	11. 990542947167034
H	6. 221813356654759	7. 246809012700198	9. 818552492398972
H	2. 344390489198614	6. 179998701852080	13. 657880089352426
H	6. 710648479003287	5. 390460414552396	11. 385893988570217
H	1. 291223283285290	9. 745848057177160	10. 411467453852982
H	5. 669162066425054	8. 981343303950007	8. 154337029390494
H	2. 931479689321105	4. 435456753073457	15. 348283391069732
H	7. 234236146099276	3. 618331227932762	12. 990998572625209
H	0. 759668123833882	11. 506455235404360	8. 803118927787731
H	5. 077514879837313	10. 721155037644344	6. 462571691660335
H	4. 546273768074117	2. 767943906945277	16. 226520013703123
H	6. 666584808906134	2. 333803007436353	15. 028960627542110
H	1. 323392906635413	12. 795743809194899	6. 765645735208711
H	3. 455373459817687	12. 379463569821091	5. 578988080240159

10 Quantum ESPRESSO Inputs

10.1 Pentacene in *p*-terphenyl

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  tprnfor= .true.
  pseudo_dir = <pseudo_dir>
  verbosity = "high"
  nstep = 256
/

&system
 ibrav = 0
  a = 1.0
  nat = 516
  ntyp = 2
  tot_charge = 0.0
  nspin = 2
  tot_magnetization = 2
  ecutwfc = 60.0
  ecutrho = 540.0
  occupations = "fixed"
  input_dft = "PBE"
  vdW_corr = "DFT-D3"
  dftd3_version = 3
/

&electrons
  electron_maxstep = 512
  mixing_beta = 0.7
  mixing_mode = "plain"
  mixing_ndim = 12
  diago_david_ndim = 8
  conv_thr = 1.0e-13
/

&ions
/

&cell
/

CELL_PARAMETERS {alat}
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  0.039614189  11.358899026   0.045139391
 -1.229319953   0.105622909  27.260950958

K_POINTS {automatic}
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ATOMIC_SPECIES
 C   -1.0  C.pbe-rrkjus.UPF
 H   -1.0  H.pbe-rrkjus.UPF

ATOMIC_POSITIONS {angstrom}
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C	11.5954652546	1.9293759078	14.3988263427
C	11.1420853872	2.9808244530	25.6950991208
C	10.8263978300	2.9799792338	14.9291451765
C	10.5195918547	4.0275815101	14.0434866382
C	11.4530667089	1.9286132940	26.5726981356
C	11.5993879413	2.9824461882	24.2858174186
C	10.3780531671	2.9871481727	16.3431860266
C	11.2049271173	3.9881313636	23.3843039927
C	10.7933791352	1.9924835054	17.2486962589
C	11.6048860855	3.9622198240	22.0525410068
C	10.3928909439	2.0112834666	18.5805675688
C	12.4191184712	2.9361101653	21.5757192276
C	9.5637519685	3.0253146134	19.0571837889
C	12.8337796230	1.9390422583	22.4559585717
C	9.1377234183	4.0181655252	18.1772985537

C	12.4267339436	1.9609428027	23.7853743015
C	9.5364188141	3.9980829536	16.8439676560
H	10.0734835376	4.8673777480	25.6089475245
H	11.8773619106	1.0819996425	15.0201228958
H	9.9381985877	4.8841089764	14.3786384222
H	12.0585340343	1.0882300999	26.2408820836
H	10.5579625181	4.8007433553	23.7076344144
H	11.4570825539	1.1921920650	16.9279209935
H	11.2636088664	4.7504237723	21.3824399310
H	10.7477306820	1.2282996614	19.2498558541
H	12.7248467874	2.9128970886	20.5306843960
H	9.2606111405	3.0449901139	20.1033621348
H	13.4848661658	1.1340782833	22.1180074163
H	8.4829527433	4.8176785298	18.5213246302
H	12.7672315475	1.1586309374	24.4349884498
H	9.1773133992	4.7923727086	16.1934460139
C	-0.3172961277	6.7929916355	14.4953868081
C	-0.5622726652	6.8559788835	26.8072612987
C	6.4505178238	11.4435838052	16.4104624885
C	5.6281052832	11.4225039133	19.1220717509
C	5.1599059236	10.4555078316	18.2344957210
C	5.5640756223	10.4683078259	16.9027128954
H	-0.0890254378	7.6752308746	15.0896727933
H	-0.0479329600	7.7434198491	26.4434520291
H	-0.3502168448	7.4997153014	17.0520765380
H	5.3219219024	11.4082682737	20.1680561095
H	4.4690446935	9.6822233114	18.5688577336
H	5.1728489317	9.6992055016	16.2406838344
C	6.6071289105	10.3658597483	14.1301276578
C	-0.7677023500	11.4314224176	25.9714621532
C	6.5100833253	10.3937927759	26.4502924353
H	6.0390633132	9.5061654968	14.4798826568
C	-0.3092094750	5.7513964021	24.5535614807
H	6.3185143158	9.5000309310	25.8604727343
C	-0.7011632925	10.3782218967	23.6807002573
C	0.5898575452	6.7250147007	24.0836245114
C	-0.3212019529	10.3871580572	22.3426650607
H	6.5630416402	9.6939630968	23.8980610117
C	1.0082324289	6.7493313828	22.7571868040
H	0.9847473494	7.4780656535	24.7615734396
C	0.5423665646	5.7942527486	21.8554507462
H	-0.6349687234	9.5663379892	21.6993955165
H	1.7111357672	7.5180242735	22.4391083312
H	0.8577215245	5.8172361263	20.8126578968
C	2.3671157578	9.7602136155	26.7267488492
C	3.7344784861	7.4937947875	14.4929795437
C	3.0913302519	8.6945544377	26.1670927171
C	2.9446268042	8.5346567280	15.0116481432
C	2.6160257110	9.5666437315	14.1157042985
C	3.3457284598	7.6021391063	27.0146337740
C	3.5429299814	8.7134202130	24.7570247277
C	2.4950354579	8.5516357929	16.4244533450
C	3.1101412103	9.7058922213	23.8587685592
C	2.9003682542	7.5611888972	17.3383216203
C	3.5126250605	9.7003094357	22.5275329347
C	2.5067419299	7.5992450130	18.6721222930
C	4.3494571897	8.6967930611	22.0451985008
C	1.6874563782	8.6260719869	19.1389433376
C	4.7979142513	7.7098230155	22.9224698942
C	1.2586362823	9.6072575022	18.2467669378
C	4.4064857299	7.7224367531	24.2563825177
C	1.6578839858	9.5713277794	16.9144000360
H	2.1364542802	10.6411903918	26.1334295954
H	4.0292492649	6.6556071003	15.1209282360
H	2.0059926052	10.4087074912	14.4363306110
H	3.8864258225	6.7310071265	26.6514806205
H	2.4304285692	10.4907896857	24.1833804385

H	3.5484419088	6.7470174816	17.0223752425
H	3.1527566965	10.4848038141	21.8635034276
H	2.8590227399	6.8203506517	19.3474917606
H	4.6404242233	8.6849219013	20.9957018117
H	1.3868697043	8.6599367946	20.1858468969
H	5.4634595117	6.9167469930	22.5838782465
H	0.6027643556	10.4114621044	18.5782888103
H	4.7893588137	6.9433846655	24.9122036040
H	1.3008243066	10.3578876626	16.2535681759
C	14.7822659154	5.7819812699	14.8816023997
C	7.4460040273	6.8603678919	26.7606028401
C	14.3802358742	11.4816080189	16.3230271433
C	14.7817875420	6.7773763592	17.1989625719
C	14.3840932229	6.7653687288	18.5322271673
C	13.5629599440	11.4554097779	19.0343237564
C	13.1451473744	10.4538582563	18.1610653903
C	13.5488722462	10.4674297045	16.8303383737
H	8.0378903462	7.7084477996	26.4234653389
H	14.7609904610	7.5359900727	19.2036772385
H	13.2570372998	11.4395639376	20.0796768029
H	12.4916793772	9.6537173884	18.5052666601
H	13.1989658577	9.6683515313	16.1817921898
C	14.5507673677	10.3916395717	14.0517431741
C	7.2130490139	11.4746109740	25.8919633963
C	14.2795810623	10.4506238229	26.3441515432
H	14.0010693882	9.5233968658	14.4091497693
C	7.5984323097	5.7971815881	24.4743149092
H	13.9894159718	9.5993022405	25.7331281622
C	7.2463967632	10.4782611884	23.5786160953
C	8.4324451560	6.8116071676	23.9701416636
C	7.6442011623	10.5000313920	22.2456440662
H	14.5159051131	9.6007141593	23.8574152368
C	8.8725144958	6.8028767854	22.6497779672
H	8.7580585223	7.6271859621	24.6116993054
C	8.4882660782	5.7802340409	21.7857694239
H	7.2778959989	9.7282461596	21.5694637581
H	9.5284896117	7.6017818412	22.3061497981
H	8.8237172147	5.7777240954	20.7495546643
C	10.4700029462	9.7649830194	26.3130135995
C	11.5934096498	7.5623166038	14.3777178939
C	11.1293287743	8.6534090813	25.7614623665
C	10.9413464934	8.6761138544	14.9355387570
C	10.7211339321	9.7641441945	14.0725347542
C	11.3269526210	7.5557856783	26.6172192744
C	11.5861988280	8.6403482247	24.3529965787
C	10.5130739991	8.7070749857	16.3532524659
C	11.1729469830	9.6284431413	23.4407188420
C	10.8492269070	7.6734082941	17.2467772819
C	11.5892469923	9.6052239989	22.1141189431
C	10.4558689614	7.7128173889	18.5802384539
C	12.4290377776	8.5929356105	21.6525212719
C	9.7157646511	8.7881060757	19.0689774246
C	12.8562312284	7.6099515679	22.5424883113
C	9.3666955076	9.8188612057	18.1986018117
C	12.4414352903	7.6342239673	23.8701429048
C	9.7583520909	9.7781230595	16.8650943423
H	10.2992205713	10.6570172569	25.7142986044
H	11.7898190012	6.6780230976	14.9800443364
H	10.2215258310	10.6630121248	14.4273845016
H	11.8202178208	6.6551058873	26.2571986120
H	10.4968288920	10.4215125961	23.7533765264
H	11.4416557162	6.8241895664	16.9127075794
H	11.2398787434	10.3826352262	21.4356580588
H	10.7426797687	6.8945824841	19.2399818285
H	12.7455170894	8.5693312206	20.6105547233
H	9.4120094000	8.8183868675	20.1146194369
H	13.5280859433	6.8180511931	22.2146545824

H	8.7689095058	10.6608144633	18.5452184304
H	12.8040503113	6.8552833720	24.5370523980
H	9.4534790495	10.5984276386	16.2189549288
C	7.3352453878	5.0448519730	12.4558741361
C	8.0000019708	6.3306902802	12.5843784842
C	6.6067554602	5.1686748491	14.8124114096
C	7.2715803970	6.4543758668	14.9411336517
C	6.6588153517	4.5056098089	13.5702163431
C	7.9495609156	6.9927029301	13.8270461744
C	8.0167241993	4.9478083504	10.1013103073
C	8.6765741116	6.2175733564	10.2242451307
C	5.9260914907	5.2855978122	17.1730676154
C	6.5867534959	6.5554492254	17.2962934090
C	7.3770847297	4.3849310368	11.2301141176
C	8.6578067131	6.8740818575	11.4790412631
C	5.9481508040	4.6272244718	15.9186694623
C	7.2321529598	7.1128740227	16.1677501380
C	7.9828789004	4.3115117414	8.8471908498
C	9.2907491073	6.7786759811	9.0844635076
C	5.3083886251	4.7270570344	18.3127775980
C	6.6136933765	7.1972223133	18.5481751054
C	8.5549162067	4.9071233602	7.7389492063
C	9.2192707086	6.1365230241	7.8585939766
C	5.3713056976	5.3751738895	19.5365703256
C	6.0327155869	6.6062289625	19.6539606679
H	6.1565830996	3.5445042989	13.4631270168
H	8.4538919295	7.9529943286	13.9296329765
H	6.8769604108	3.4227780255	11.1213163074
H	9.1548568362	7.8395640696	11.5773975045
H	5.4539904674	3.6603659633	15.8199162997
H	7.7380674238	8.0717521832	16.2755415443
H	7.4795873778	3.3514263327	8.7626682904
H	9.8079681202	7.7334747939	9.1791222226
H	4.7918479286	3.7715261192	18.2196558597
H	7.1193595905	8.1567094666	18.6329403309
H	8.4706650022	4.4268760299	6.7685509883
H	9.6718296549	6.5868805775	6.9785276720
H	4.9208579619	4.9276341062	20.4188427876
H	6.1090035256	7.0905269617	20.6223609333

10.2 Pentacene in benzoic acid

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&control
  prefix = <prefix>
  calculation = "scf"
  tprnfor = .true.
  pseudo_dir = <pseudo_dir>
  verbosity = "high"
  nstep = 256
/
```

```
&system
  ibrav = 0
  a = 1.0
  nat = 366
  ntyp = 3
  tot_charge = 0.0
  nspin = 2
  tot_magnetization = 2
  ecutwfc = 60.0
  ecutrho = 540.0
  occupations = "fixed"
  input_dft = "PBE"
  vdW_corr = "DFT-D3"
```

```

dftd3_version = 3
/

&electrons
  electron_maxstep = 512
  mixing_beta = 0.7
  mixing_mode = "plain"
  mixing_ndim = 12
  diago_david_ndim = 8
  conv_thr = 1.0e-13
/

&ions
/

&cell
/

CELL_PARAMETERS {alat}
  11.076933597  0.012082594 -0.022398036
    0.016755706  15.194499591  0.065683443
   -3.078174263  0.090345760  21.654310410

K_POINTS {automatic}
  1 1 1  0 0 0

ATOMIC_SPECIES
  C  -1.0  C.pbe-rrkjus.UPF
  H  -1.0  H.pbe-rrkjus.UPF
  O  -1.0  O.pbe-rrkjus.UPF

ATOMIC_POSITIONS {angstrom}
O      1.1638515896      1.0926929211      0.2898086990
O      4.8319913267      0.6249781236      1.4555287656
C      0.4107079846      1.2870593964      1.2685640211
C      0.7123568480      2.3247785322      2.2797142960
C      1.8590683430      3.1148488831      2.1335159237
C      2.1517702782      4.0922777161      3.0800579082
C      1.3087702828      4.2811945422      4.1758514221
C      0.1651156213      3.4945289633      4.3224684985
C     -0.1349791530      2.5219127497      3.3772556674
H      2.5110132689      2.9651575713      1.2742001577
H      3.0372306793      4.7130670504      2.9524307401
H      1.6136016978     -0.0514320282      4.8880036363
H     -0.4979309386      3.6481219132      5.1727824082
H      4.4424189739      1.9730874019      3.4011516607
H      4.6952450678     -0.1280685533      0.7409167293
O      2.7838935477      3.6515979780     10.5049119465
O      1.2926063162      3.9382546465     21.4588788854
O     -0.3487128932      1.3352005064     11.0763334781
O     -0.6999013728      3.1462832115      9.3358393554
O     -2.3569457240      4.4092361814     20.2799439487
O      3.2396275900      1.8746611596     12.2586979221
C      3.5675827853      3.8748222649      9.5591093582
C      2.0373375671      3.7291858692     20.4764251702
C     -1.1419318138      1.1432043092     12.0234584723
C      3.2805718456      4.9150351574      8.5462325990
C      1.7161623037      2.6900130638     19.4724336113
C     -0.8563484804      0.1419886681     13.0742546355
C      2.1715243006      0.6144646640      8.6721136735
C      0.5622215961      1.9125128250     19.6332260415
C      0.2327270268      4.3354470648     12.9033462537
C      1.8949735933      1.5740087802      7.7024758279
C      0.2524863889      0.9298614593     18.6974655466
C      0.5269235105      3.3545194757     13.8450473701
C      2.7663697103      1.7571972186      6.6282349849
C      1.0870481882      0.7208844675     17.5993892572

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C	-0.2599461511	3.2236639506	14.9902572832
C	3.9219259478	0.9815533368	6.5268490419
C	2.2359387754	1.4961974500	17.4370443910
C	-1.3477519865	4.0739938144	15.1930868385
C	4.2042644559	0.0259036622	7.4939939367
C	2.5524778040	2.4765162983	18.3690633472
C	-1.6426107287	5.0586890545	14.2591199308
H	1.4987018929	0.4669522691	9.5154331295
H	-0.0856994541	2.0786562117	20.4924714058
H	0.8375545002	4.4346358797	12.0034004522
H	0.9988325744	2.1851673194	7.7941205103
H	-0.6403372156	0.3221670654	18.8335639449
H	1.3703221147	2.6876620355	13.6756911190
H	2.5432787949	2.5090294597	5.8710485750
H	0.8788286862	5.0950675717	16.7972835564
H	-0.0254233833	2.4531113126	15.7248850744
H	4.6097636319	1.1286299814	5.6954981962
H	2.8912794800	1.3272449717	16.5839551264
H	-1.9734389084	3.9635650800	16.0773735124
H	-0.1262513826	4.6758124077	7.5554695421
H	-2.0148345858	3.0726773212	18.3121853989
H	2.8839536372	0.5752375243	14.2464700993
H	-0.5803849986	2.4228538515	10.0811400136
H	-2.2047952810	5.1468561125	21.0010955980
H	3.0820290996	2.5893059784	11.5132291216
O	6.7105045624	1.0980721477	0.2908573033
O	10.3860576845	0.6119941620	1.4588555639
C	5.9422242262	1.3008644803	1.2567035201
C	6.2366823137	2.3378584533	2.2698972384
C	7.4049200482	3.1018342964	2.1576276930
C	7.6885920928	4.0752980915	3.1109567342
C	6.8127269270	4.2870406779	4.1765564137
C	5.6474770645	3.5274832287	4.2872589958
C	5.3575388317	2.5574784652	3.3369617886
H	8.0811574081	2.9323318872	1.3211093078
H	8.5932843920	4.6740442617	3.0146773367
H	7.1640855841	0.0050975319	4.8431828246
H	4.9559581466	3.6979408542	5.1109467290
H	10.0437795851	1.9271193010	3.4480303515
H	10.2450465796	-0.1333113563	0.7391930868
O	8.4390164927	3.6291706405	10.3805425400
O	6.8719991509	3.9380621924	21.4653843129
O	5.1098249980	1.3858186314	11.0866247016
O	4.6983950666	3.2220184447	9.3786421209
O	3.1482717281	4.4009152985	20.2557613279
O	8.8026200446	1.8115450436	12.1431377267
C	9.2455346121	3.8148571336	9.4441789000
C	7.6149146221	3.7395655286	20.4798017503
C	4.3520758128	1.1991511451	12.0638127699
C	8.9807001701	4.8169531850	8.3864038228
C	7.3016289379	2.7045908052	19.4688607550
C	4.6560016361	0.1797323653	13.0927371059
C	7.6998129272	0.6553943316	8.6544613763
C	6.1418563902	1.9314049713	19.6065403166
C	7.4278698550	1.5992256573	7.6690489577
C	5.8407514037	0.9592122409	18.6566963202
C	8.3083000517	1.7700092365	6.5998586751
C	6.6901754555	0.7548014374	17.5686321498
C	9.4662300522	0.9949352086	6.5178832915
C	7.8484837464	1.5211968087	17.4336074694
C	9.7461013543	0.0549460438	7.5006064401
C	8.1542029151	2.4924038869	18.3780811748
H	7.0216077681	0.5183963610	9.4955520446
H	5.4846675292	2.0904288655	20.4602457960
H	6.5289756353	2.2085436859	7.7470052355
H	4.9440968745	0.3528910148	18.7761742116
H	8.0917658621	2.5123096716	5.8312803025

H	6.3878991967	5.0410740852	16.8397146862
H	10.1603881998	1.1326079440	5.6908662666
H	8.5211839811	1.3569329323	16.5923316549
H	4.9797239108	4.4246365914	7.3236649693
H	3.4520470932	3.0785578941	18.2594205946
H	8.4292706836	0.5655565580	14.1698374473
H	4.8377381235	2.4824967882	10.1035928862
H	3.3071641995	5.1380265628	20.9762820596
H	8.6756306471	2.5230129879	11.3954948560
O	1.1595664335	6.1747251818	0.3125327417
O	1.1664068195	11.2229539155	0.3006202412
O	4.8181915519	5.7045572892	1.4820598324
O	4.8809189496	10.7358694523	1.5270657157
C	0.4136324527	6.3816498191	1.2935778451
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