

Supporting Information

Singlet Fission in Carbene-Derived Diradicaloids

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Table of Contents

Section S1. Spectroscopical Methods – General	S3
Section S 2. Steady State Spectroscopy	S4
Section S 3. Femtosecond Transient Absorption Spectroscopy	S6
Section S 4. Nanosecond Transient Absorption Spectroscopy	S14
Section S 5. Computational Details – General	S18
Section S 6. Configuration State Functions (CSFs)	S21
Section S 7. Diabatic Electronic States	S46
Section S 8. XYZ Coordinates	S54
Section S 9. Supplementary References	S81

Section S1. Spectroscopical Methods – General

All compounds were prepared as reported previously.¹ For the photophysical studies, samples were prepared in a glove box under inert atmosphere (argon- or dinitrogen) and placed in subsequently sealed cuvettes with different path lengths (depending on the chosen concentration). For low temperature measurements, cuvettes were placed in a liquid dinitrogen cryostat (Oxford Instruments: Optistat DN). 3-Methylpentane was used as solvent, since it forms an optical transparent glass at cryogenic temperatures. It was dried, degassed and purified by distillation over potassium under inert atmosphere. All investigated compounds did not show any signs of decomposition in solution over the course of more than a month.

Steady state absorption spectra were recorded by using a Varian Cary 5000 spectrometer. Steady state fluorescence spectra in the NIR were measured with a Horiba FluoroMax3. The excitation wavelength was set to 670 nm.

All fs- and nsTA spectra were carried out with an amplified Ti:Sapphire CPA 2110 fs laser system (Clark MXR: output 775 nm, repetition rate 1 kHz, 150 fs pulse duration) using a customized TA pump/probe detection system (Ultrafast systems: Helios, Eos). The excitation pulses at 550, 670 and 850 nm were generated *via* non-collinear parametric amplification (NOPA) and energy per pulse was reduced to 100 and 200 nJ, respectively.

Triplet-triplet sensitization experiments were performed with anthracene, purchased from a common supplier and further purified by sublimation. As excitation wavelength the second harmonic of the fundamental laser wavelength was used and reduced to an energy per pulse of 400 and 600 nJ, respectively.

All fs- and nsTA data were fitted *via* global analysis, performed with the open-source software package GloTarAn. Therefore, a sequential kinetic model was applied to fit the data. The dispersion of the instrument response function was modeled and taken into account.

Section S2. Steady State Spectroscopy

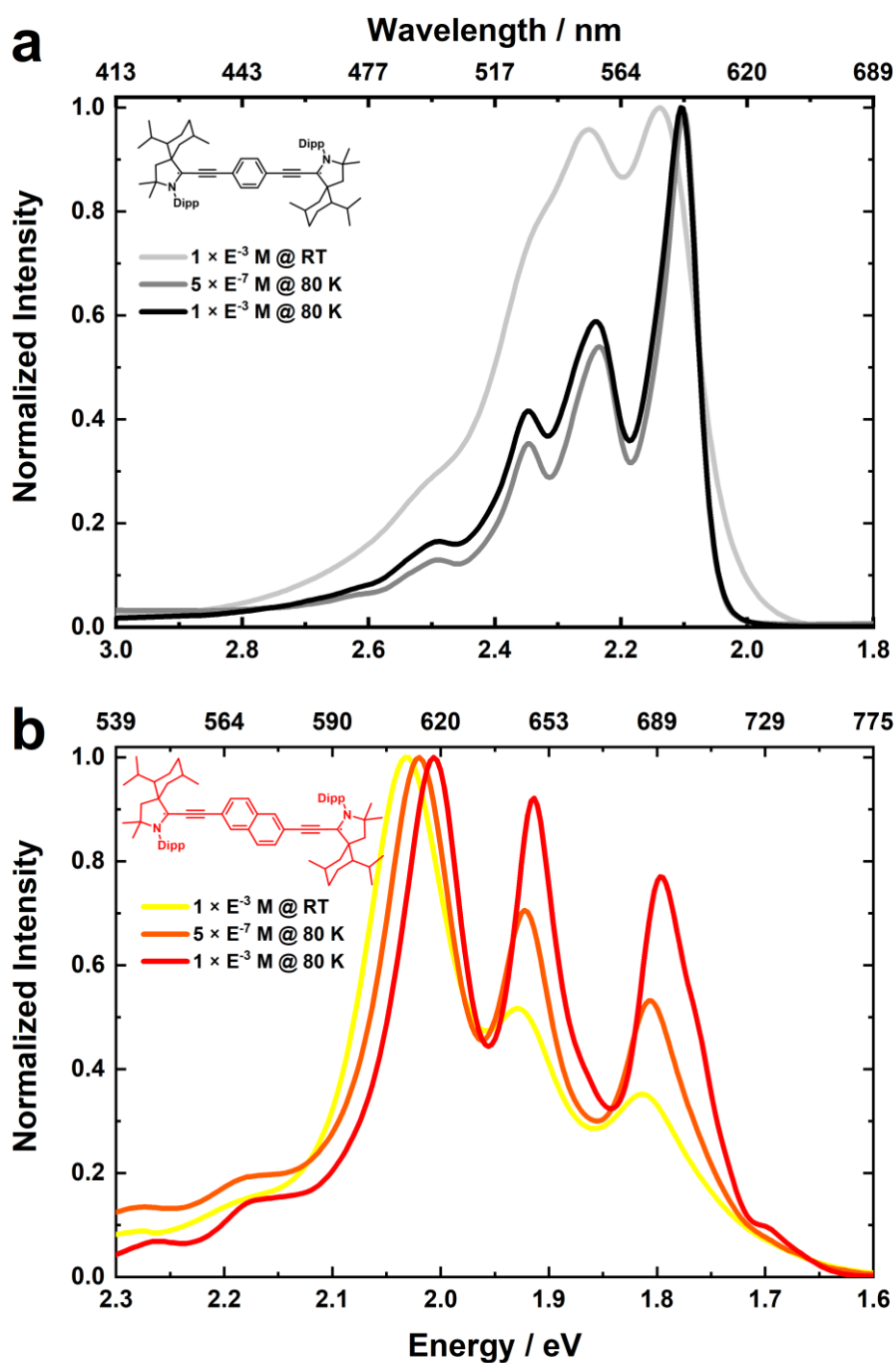


Figure S1: **a**, Normalized steady-state absorption spectra of **1** at room temperature and high concentration (1×10^{-3} M, white) as well as 80 K measured at low concentration (5×10^{-7} M, grey) and high concentration (1×10^{-3} M, black). **b**, Normalized steady-state absorption spectra of **2** at room temperature and high concentration (1×10^{-3} M, yellow) as well as 80 K measured at low concentration (5×10^{-7} M, orange) and high concentration (1×10^{-3} M, red).

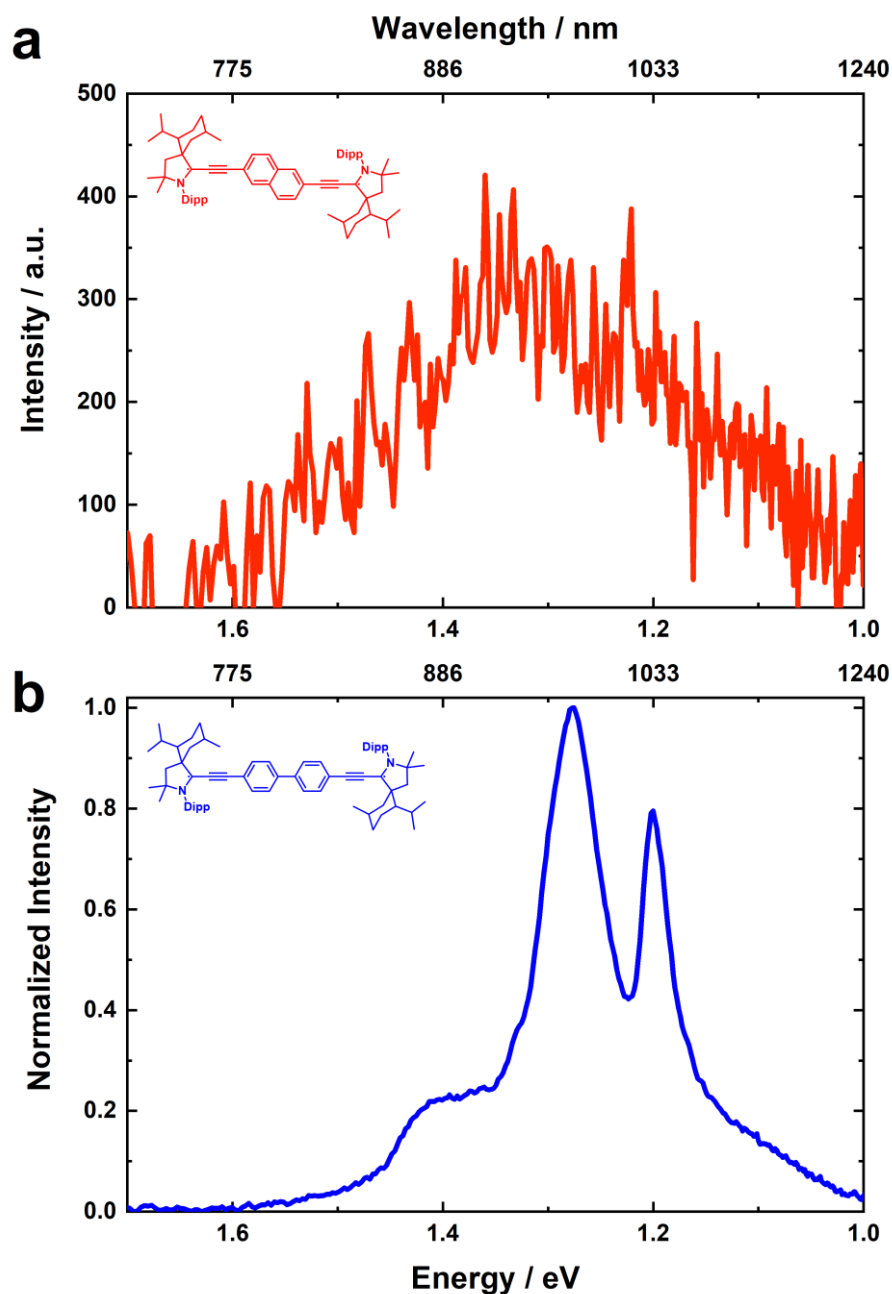


Figure S2: **a**, Steady-state fluorescence spectra of **2** measured at room temperature and concentration of 5×10^{-7} M upon excitation at 670 nm. **b**, Normalized steady-state fluorescence spectra of **3** measured at room temperature and concentration of 5×10^{-7} M upon photoexcitation at 670 nm.

Section S3. Femtosecond Transient Absorption Spectroscopy

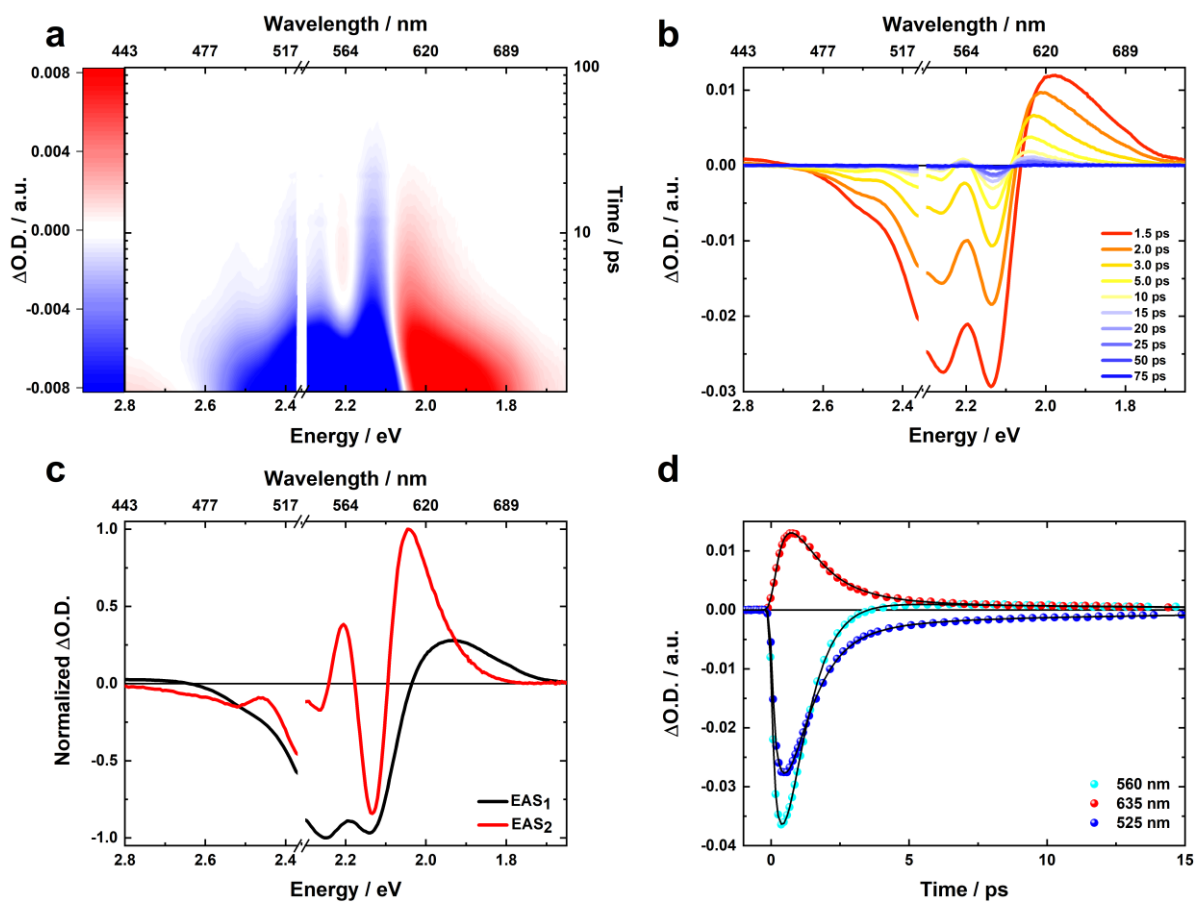


Figure S3: **a**, Zero point and chirp corrected fsTA heat map in the visible part of the optical spectrum of **1** obtained at room temperature upon photoexcitation at 530 nm and concentration of 1×10^{-3} M. **b**, Corresponding spectral slices illustrating the excited state dynamics. **c**, Evolution associated spectra obtained by global analysis. **d**, Single wavelength kinetics at 525 (cyan), 560 (blue) and 635 nm (red) as well as fit to the data (black line).

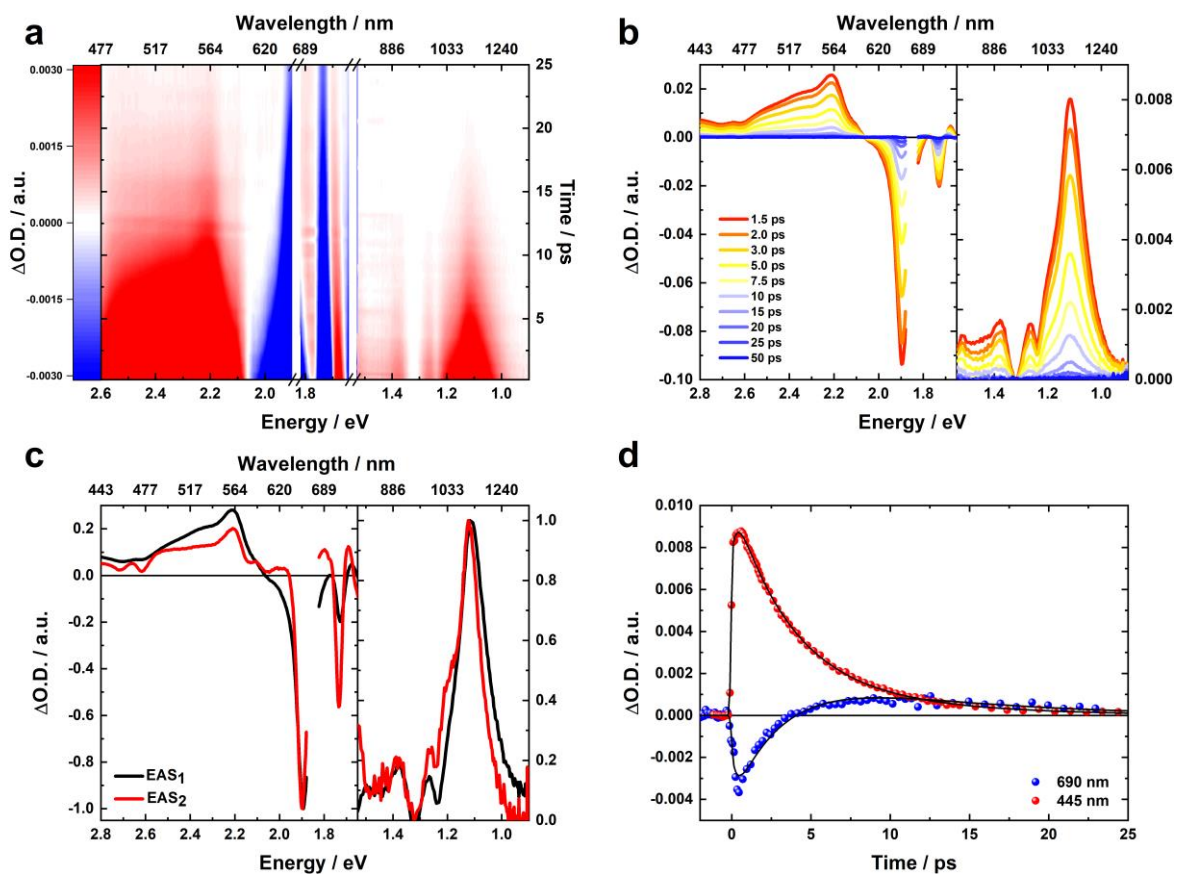


Figure S4: **a**, Zero point and chirp corrected fsTA heat map in the visible and near-infrared part of the optical spectrum of **3** obtained at room temperature upon photoexcitation at 670 nm and concentration of 1×10^{-3} M. **b**, Corresponding spectral slices illustrating the excited state dynamics. **c**, Evolution associated spectra obtained by global analysis. **d**, Single wavelength kinetics at 445 (red) and 690 nm (blue) as well as fit to the data (black line).

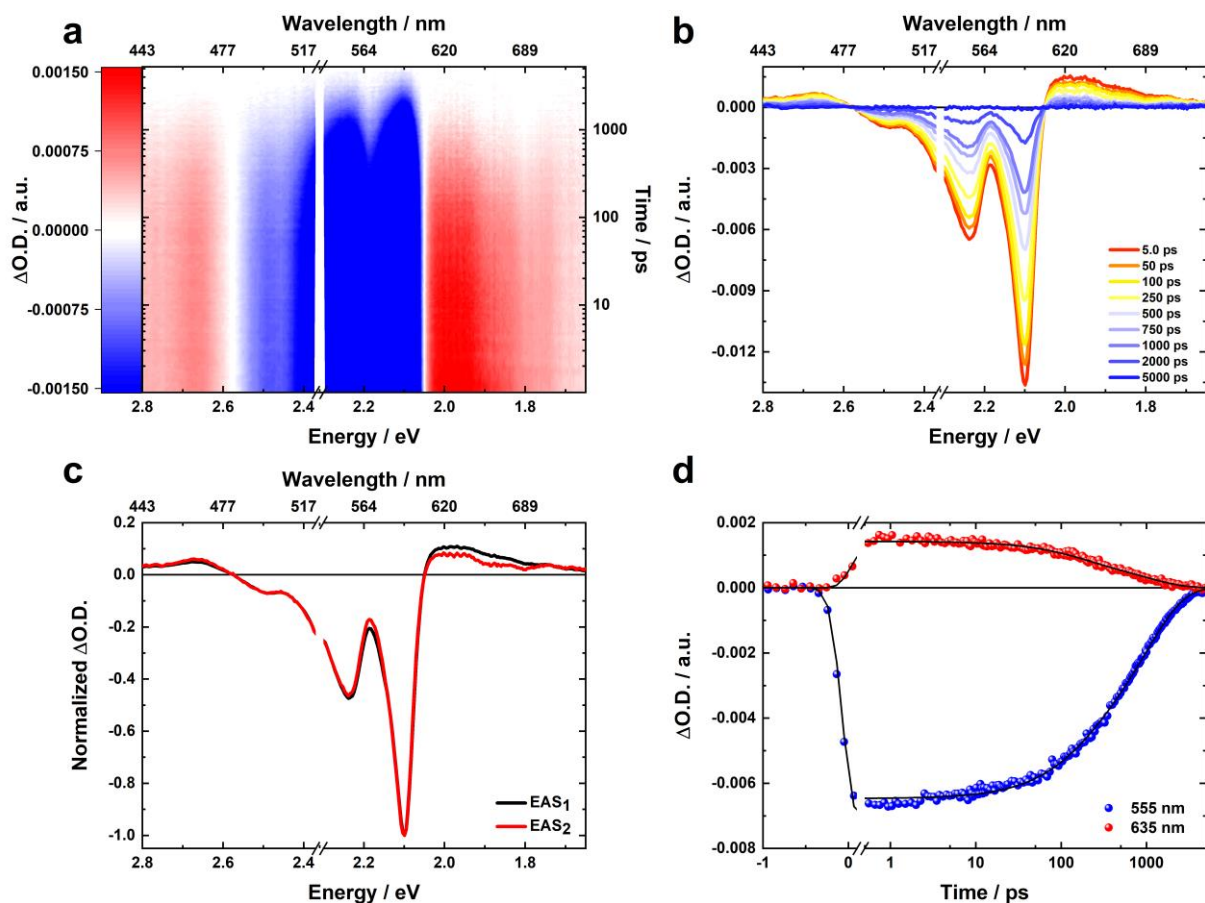


Figure S5: **a**, Zero point and chirp corrected fsTA heat map in the visible part of the optical spectrum of **1** obtained at 80 K upon photoexcitation at 670 nm and concentration of 5×10^{-6} M. **b**, Corresponding spectral slices illustrating the excited state dynamics. **c**, Evolution associated spectra obtained by global analysis. **d**, Single wavelength kinetics at 555 nm (blue) and 635 nm (red) as well as fit to the data (black line).

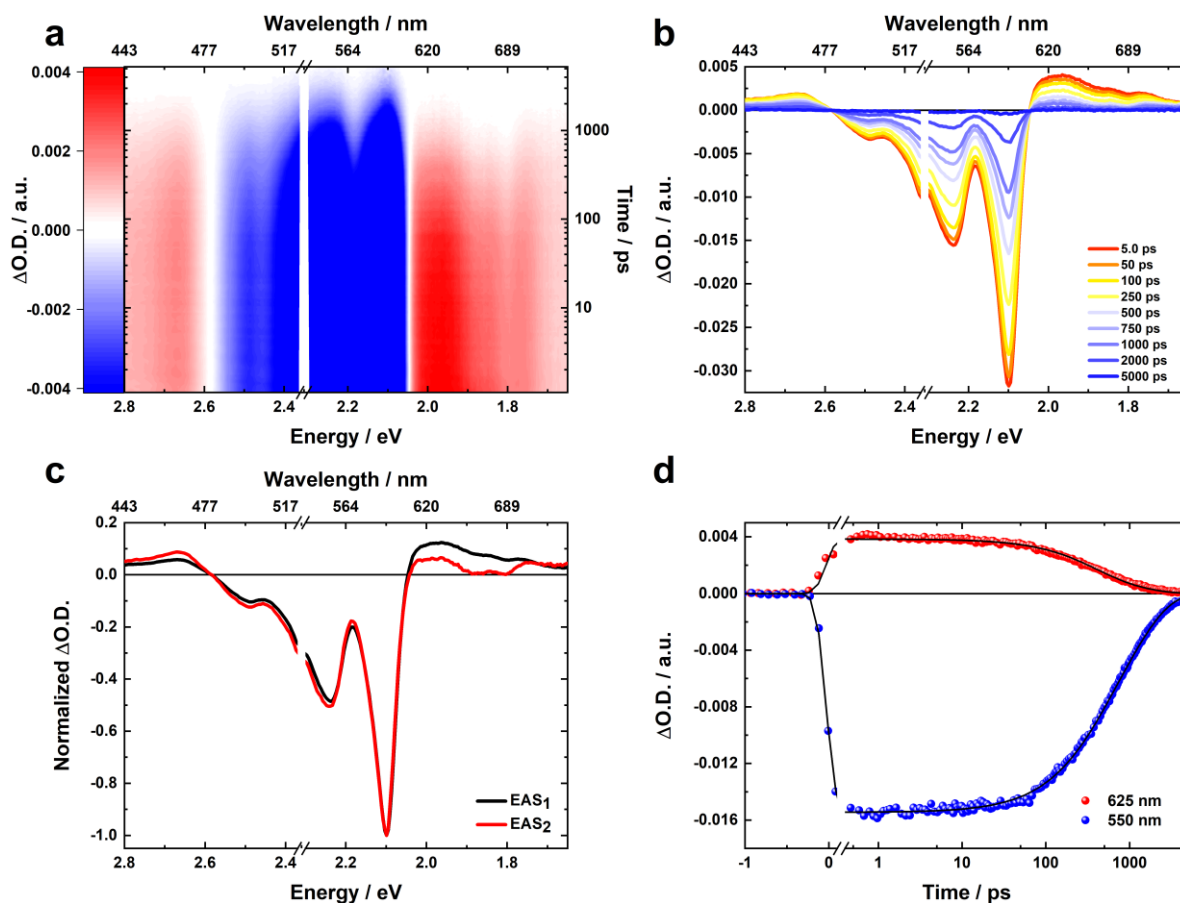


Figure S6: **a**, Zero point and chirp corrected fsTA heat map in the visible part of the optical spectrum of **1** obtained at 80 K upon photoexcitation at 670 nm and concentration of 1×10^{-3} M. **b**, Corresponding spectral slices illustrating the excited state dynamics. **c**, Evolution associated spectra obtained by global analysis. **d**, Single wavelength kinetics at 550 (blue) and 625 nm (red) as well as fit to the data (black line).

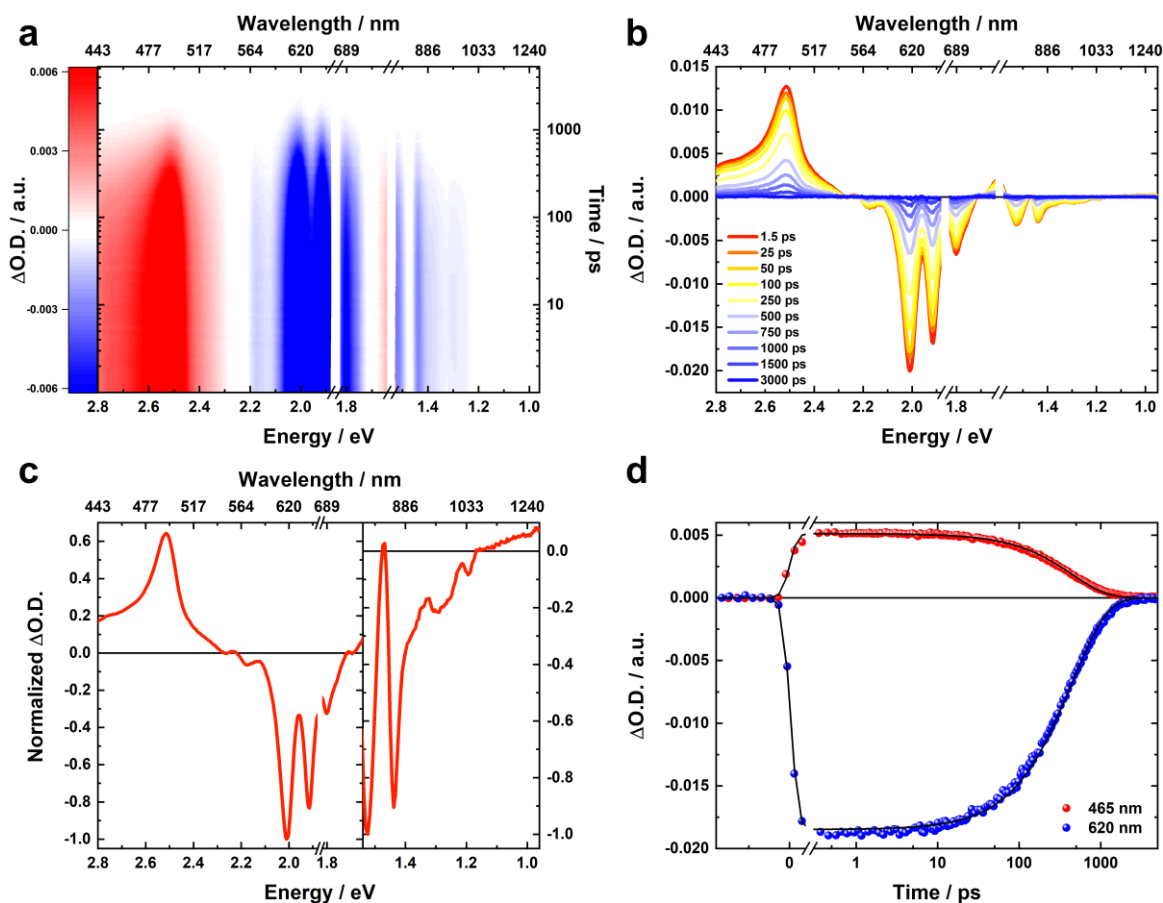


Figure S7: **a**, Zero point and chirp corrected fsTA heat map in the visible and near-infrared part of the optical spectrum of **2** obtained at 80 K upon photoexcitation at 670 nm and concentration of 5×10^{-6} M. **b**, Corresponding spectral slices illustrating the excited state dynamics. **c**, Evolution associated spectrum obtained by global analysis. **d**, Single wavelength kinetics at 465 nm (red) and 620 nm (blue) as well as fit to the data (black line).

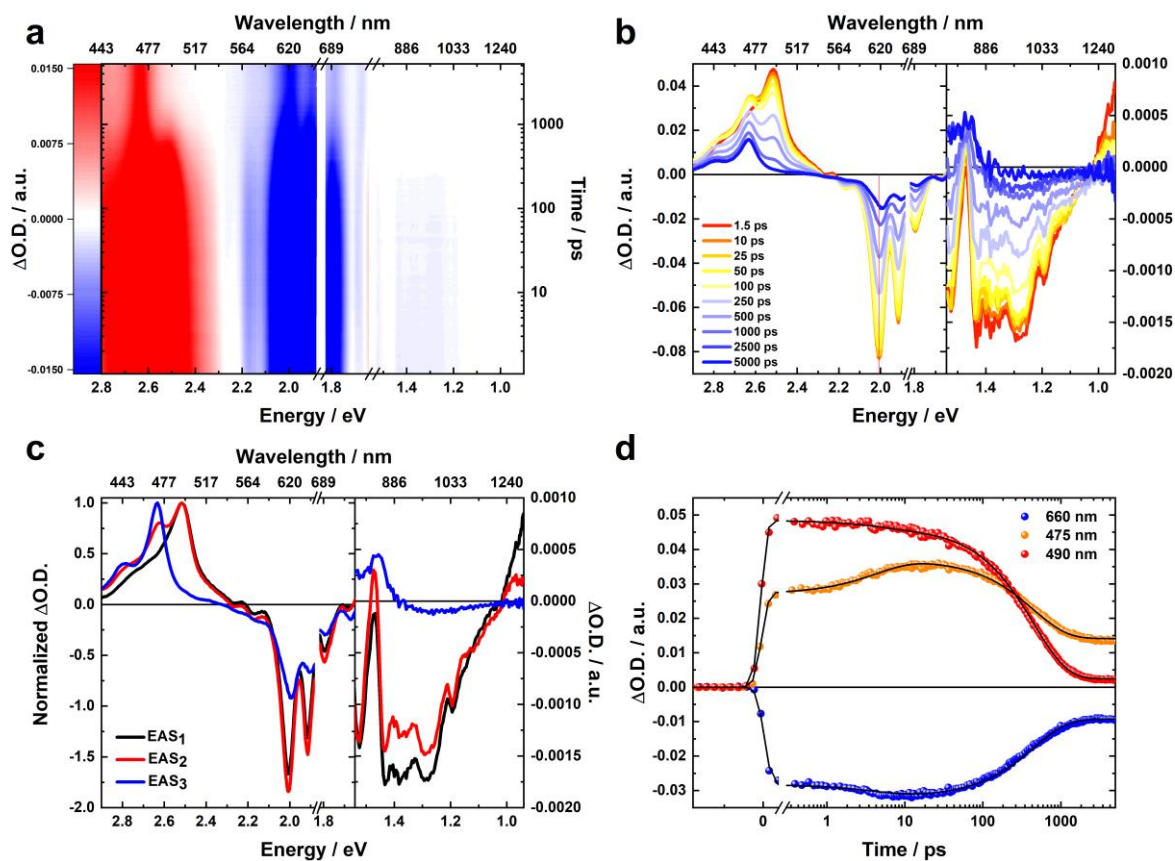


Figure S8: **a**, Zero point and chirp corrected fsTA heat map in the visible and near-infrared part of the optical spectrum of **2** obtained at 80 K upon photoexcitation at 670 nm and concentration of 1×10^{-3} M. **b**, Corresponding spectral slices illustrating the excited state dynamics. **c**, Evolution associated spectrum obtained by global analysis. **d**, Single wavelength kinetics at 475 (orange), 490 (red) and 660 nm (blue) as well as fit to the data (black line).

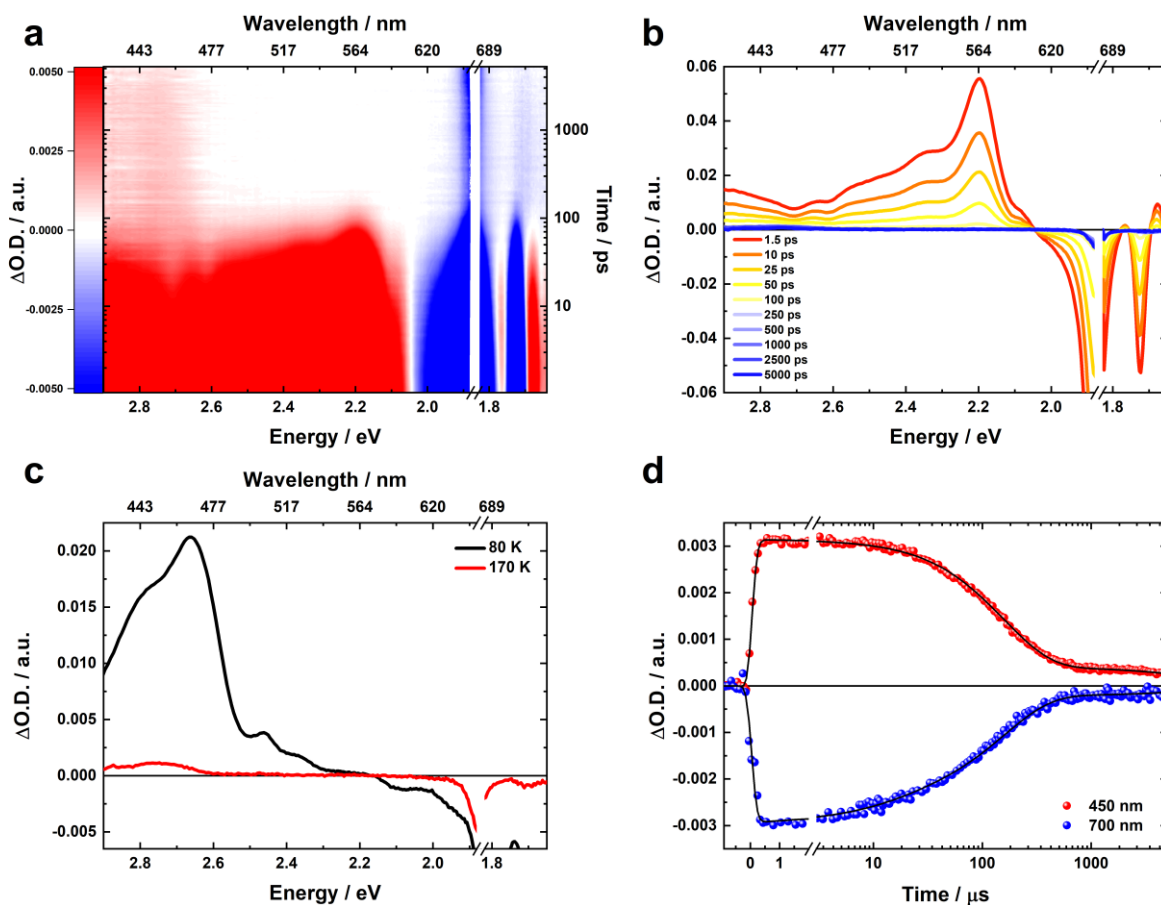


Figure S9: **a**, Zero point and chirp corrected fsTA heat map in the visible and near-infrared part of the optical spectrum of **3** obtained at 80 K upon photoexcitation at 670 nm and concentration of 1×10^{-3} M. **b**, Corresponding spectral slices illustrating the excited state dynamics. **c**, Spectral slices at a time delay of 1000 ps obtained at 80 (black) and 170 K (red). **d**, Single wavelength kinetics at 450 (red) and 700 nm (blue) as well as fit to the data (black line).

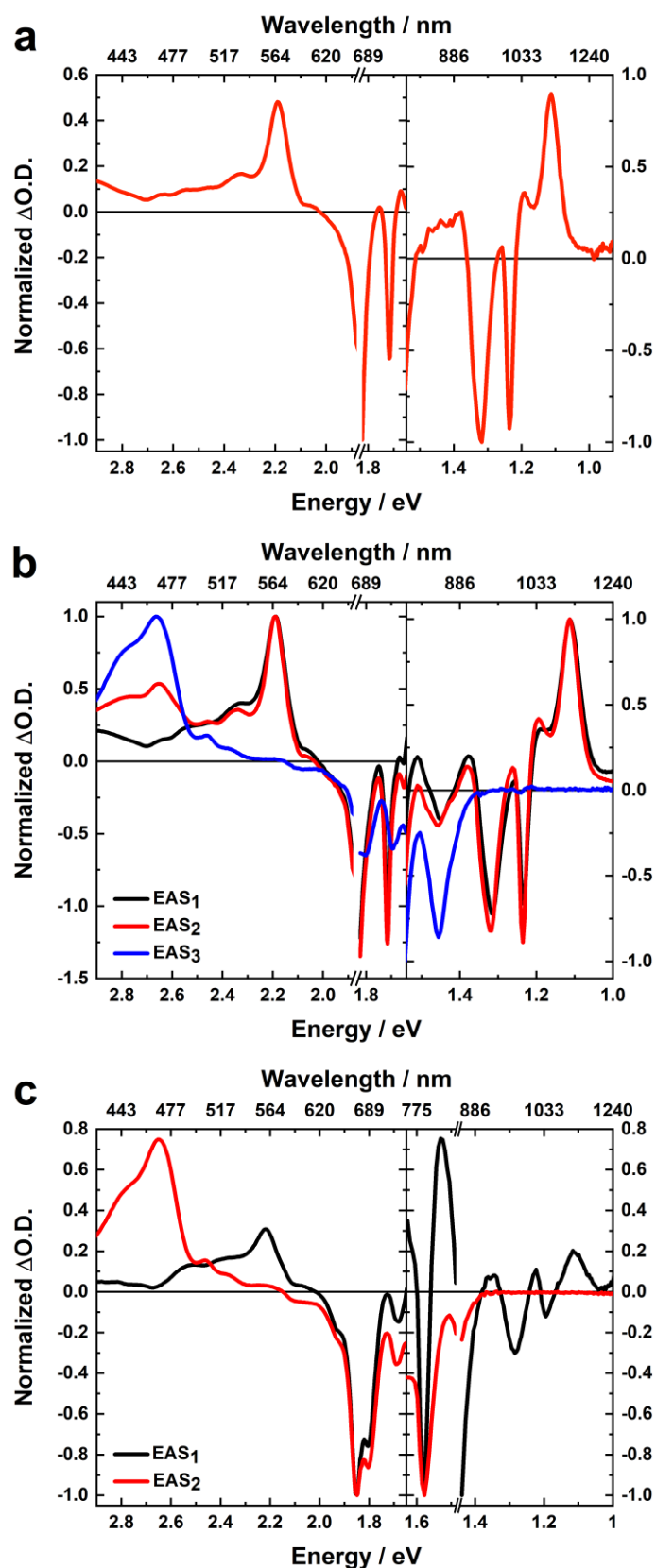


Figure S10: **a**, Evolution associated spectra of **3** obtained by global analysis at 80 K upon photoexcitation at 670 nm and concentration of 5×10^{-6} M. **b**, Evolution associated spectra of **3** obtained by global analysis at 80 K upon photoexcitation at 670 nm and concentration of 1×10^{-3} M. **c**, Evolution associated spectra of **3** obtained by global analysis at 80 K upon photoexcitation at 850 nm and concentration of 1×10^{-3} M.

Section S4. Nanosecond Transient Absorption Spectroscopy

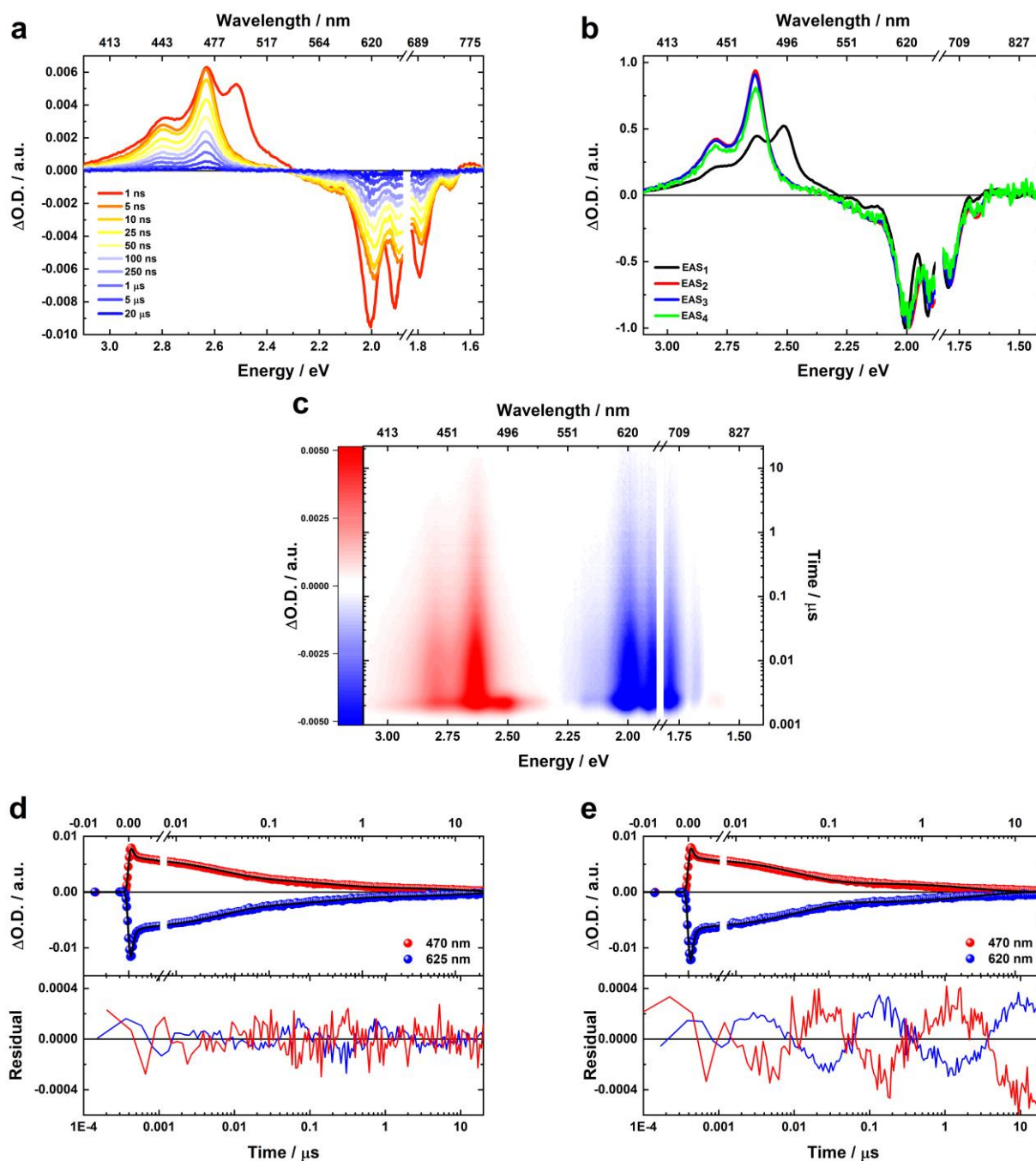


Figure S11: **a**, nsTA spectral slices in the visible part of the optical spectrum of **2** obtained at 80 K upon photoexcitation at 670 nm and concentration of 1×10^{-3} M. **b**, Evolution associated spectrum obtained by global analysis. **c**, Corresponding nsTA heat map. **d**, Single wavelength kinetics at 470 (red) and 625 nm (blue) as well as fit to the data (black line) obtained by global analysis with four kinetic components. **e**, Single wavelength kinetics at 470 (red) and 625 nm (blue) as well as fit to the data (black line) obtained by global analysis with three kinetic components. Comparison of the residuals in **d,e** reveals the necessity of four kinetic parameters to describe the deactivation kinetics of **2** in the ns time domain.

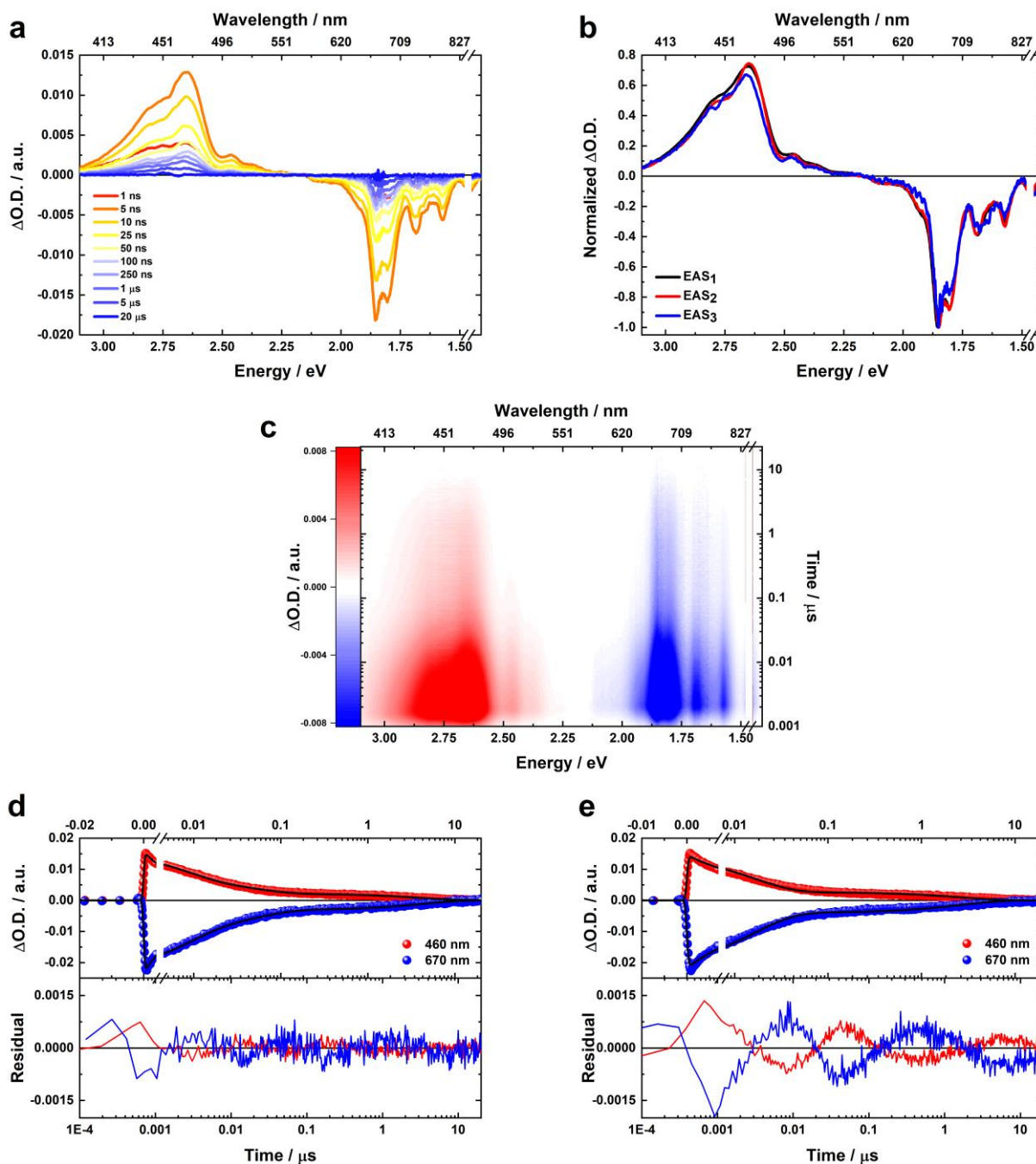


Figure S12: **a**, nsTA spectral slices in the visible part of the optical spectrum of **3** obtained at 80 K upon photoexcitation at 850 nm and concentration of 1×10^{-3} M. **b**, Evolution associated spectrum obtained by global analysis. **c**, Corresponding nsTA heat map. **d**, Single wavelength kinetics at 460 (red) and 670 nm (blue) as well as fit to the data (black line) obtained by global analysis with three kinetic components. **e**, Single wavelength kinetics at 460 (red) and 670 nm (blue) as well as fit to the data (black line) obtained by global analysis with two kinetic components. Comparison of the residuals in **d,e** reveals the necessity of three kinetic parameters to describe the triplet deactivation of **3** in the ns time domain.

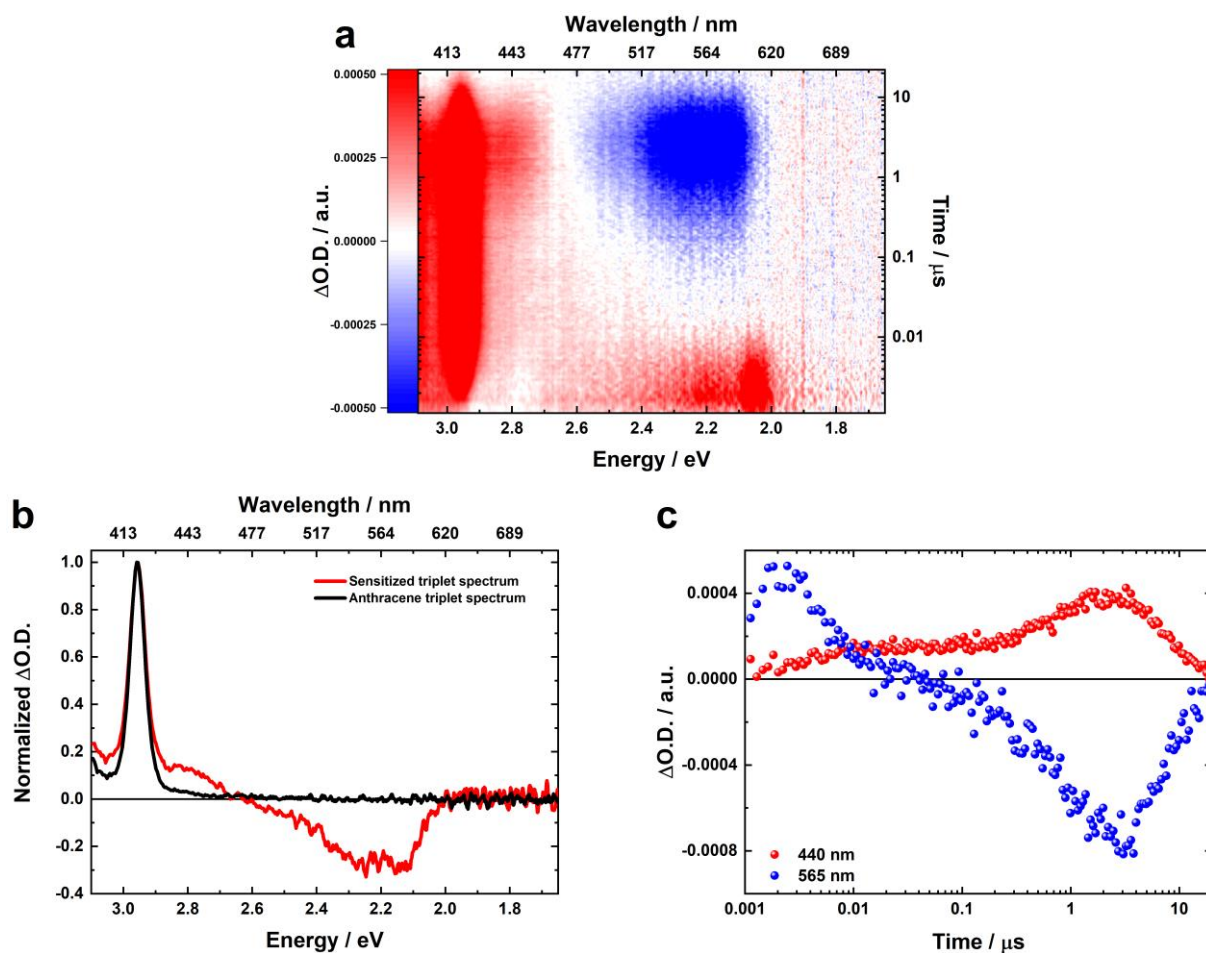


Figure S13: **a**, nsTA heat map in the visible part of the optical spectrum of the triplet-triplet sensitization experiment of **1** (3×10^{-5} M) with anthracene (8×10^{-5} M) obtained at room temperature upon photoexcitation at 387 nm. **b**, Normalized TA spectra of anthracene (black) and sensitized triplet (red) obtained at a time delay of 2.2 μs . **c**, Corresponding single wavelength kinetics at 440 (red) and 670 nm (blue).

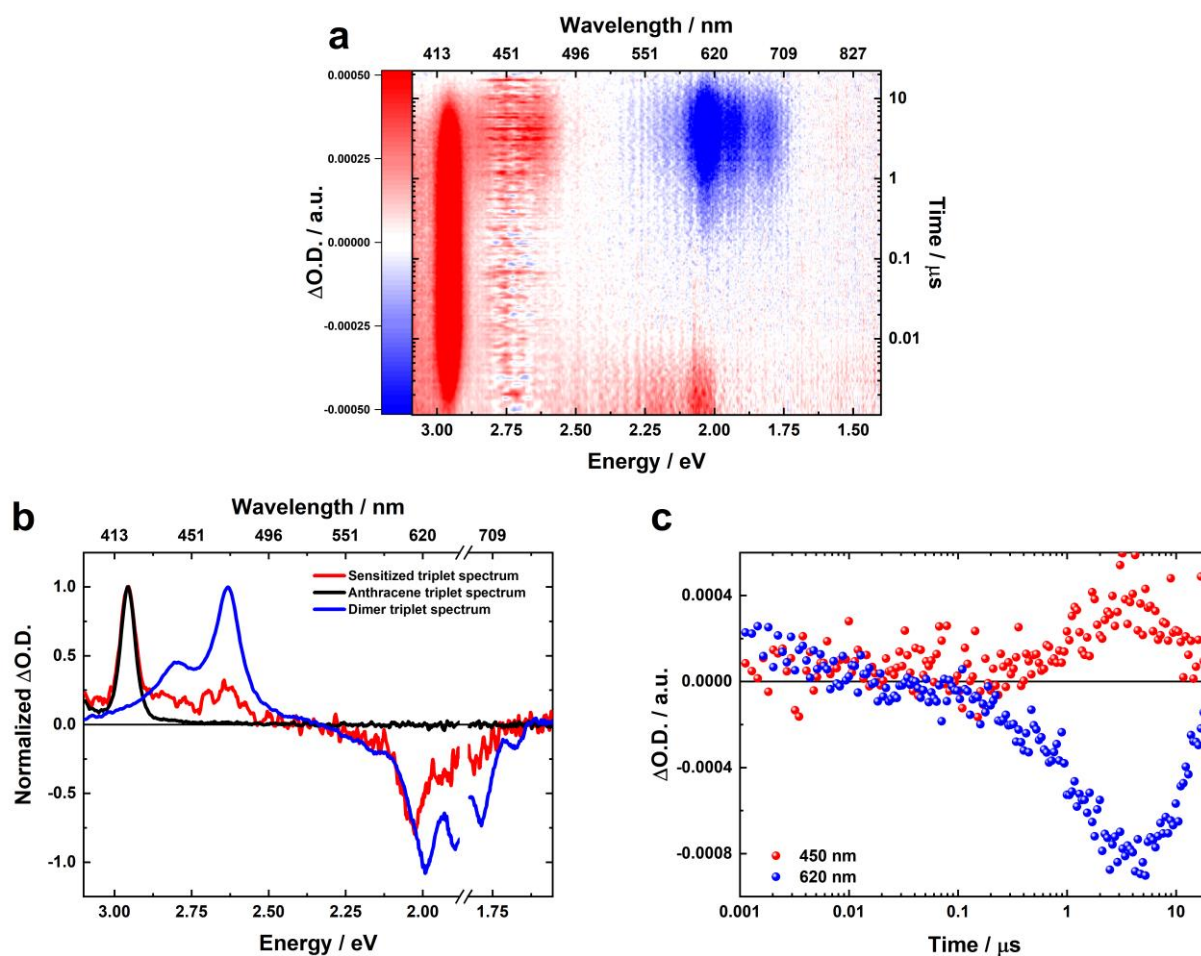


Figure S14: **a**, nsTA heat map in the visible part of the optical spectrum of the triplet-triplet sensitization experiment of **2** (3×10^{-5} M) with anthracene (8×10^{-5} M) obtained at room temperature upon photoexcitation at 387 nm. **b**, Normalized TA spectra of anthracene (black) and sensitized triplet (red) obtained at a time delay of 2.2 μs . **c**, Corresponding single wavelength kinetics at 450 nm (red) and 620 nm (blue).

Section S5. Computational Details – General

The molecular geometries were optimized using ORCA 4.0.1² with the B3LYP hybrid functional³⁻⁶ in conjunction with Grimme's 3rd generation atom-pairwise dispersion correction⁷ including Becke–Johnson damping⁸ (D3BJ) starting from the structural parameters as obtained from the solid state structures of the monomers.¹ For the optimization, the singlet multiplicity was chosen, which led to better agreement with the solid state structures than the triplet multiplicity.⁹ For the dimers, the structural parameters of the singlet, triplet and quintet multiplicities were optimized. In all geometry optimization, the def2-SVP basis set,¹⁰ the resolution of identity and chain of spheres approximation^{11,12} (RIJCOSX) and the related auxiliary basis sets¹³ (def2/J) were used. Tighter than default convergence criteria (tightopt, tightscf) as well as finer than default grid values (grid7, finalgrid7, gridx6) were applied. Test calculations with the PBE0 functional led to comparable results.

The complete active-space self-consistent-field¹⁴ (CASSCF) calculations were performed on truncated DFT-optimized structures (menthyl and Dipp groups were replaced by methyl groups; the position of the hydrogen atoms were optimized with restrained positions for all other atoms). The ZORA approximation¹⁵⁻¹⁷ was employed along with the ZORA-def2-TZVPP basis sets^{10,18} and the related auxiliary basis set¹⁹ (SARC/J). Test calculations with OpenMolcas led to comparable results as obtained with ORCA. For the state-averaged sa-CASSCF calculations, various number of roots (quintet: 1–2; triplet 3–5; singlet 5–20) and active spaces (4e/4o; 8e/8o; 12e/12o) were calculated. The same weight was applied to all roots. Second-order perturbation theory NEVPT2 including the treatment of all the core electrons (nofrozencore) was applied to account for dynamic electron correlation.²⁰ Quasi-degenerate perturbation theory (QDPT) was used to calculate model pin-orbit coupling. Calculated molecular structures and molecular orbitals were visualized with Avogadro 1.1.1, IboView and CYLView 1.0b.²¹⁻²³

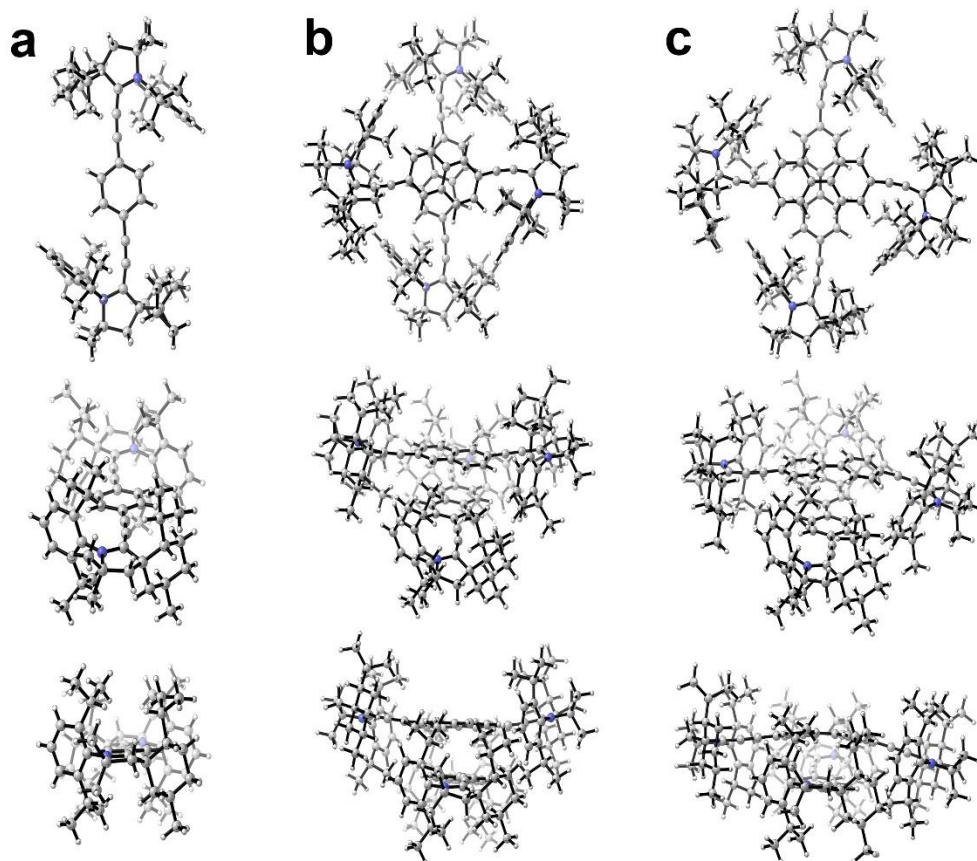


Figure S15: Optimized structures of **a**, phenyl bridged compound 1^{monomer} , **b**, 2^{dimer} and **c**, 3^{dimer} .

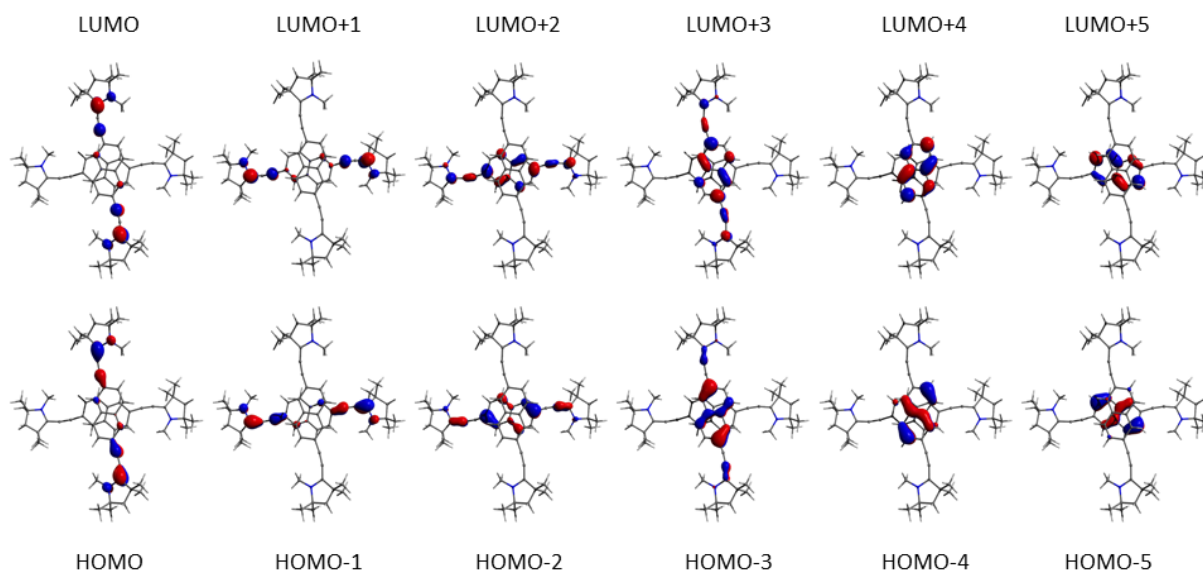


Figure S16: sa-CASSCF optimized orbitals of 2^{dimer} from state averaged calculation (singlet geometry, four singlet roots, four triplet roots and two quintet roots).

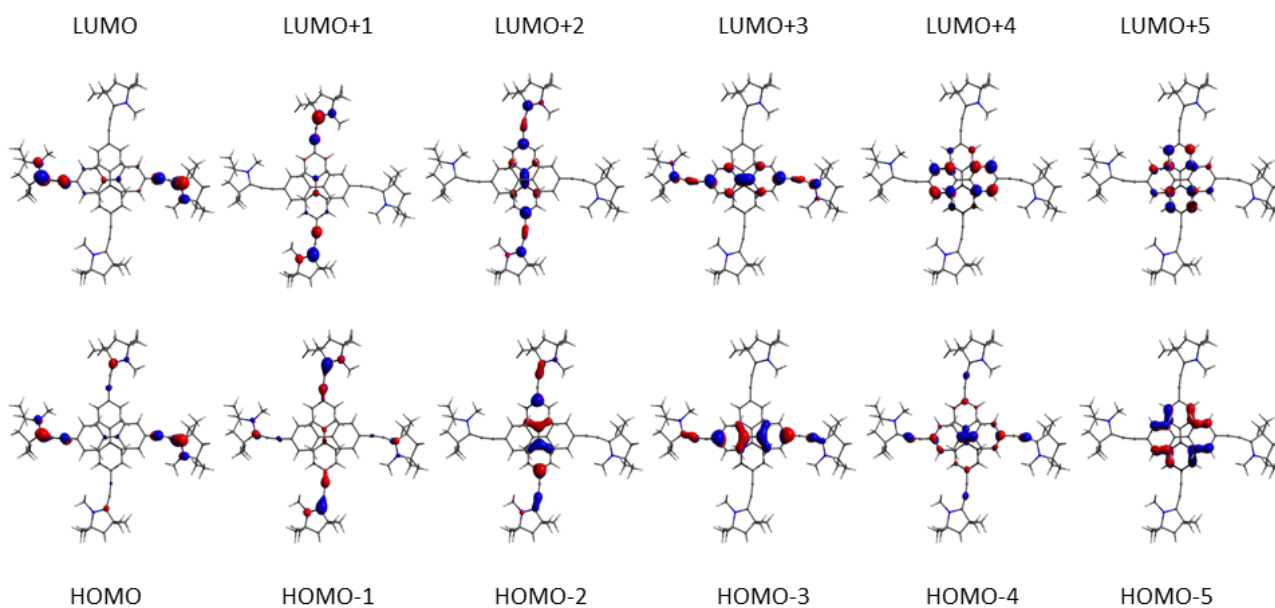


Figure S17: sa-CASSCF optimized orbitals 3^{dimer} from state averaged calculation (singlet geometry, four singlet roots, four triplet roots and two quintet roots).

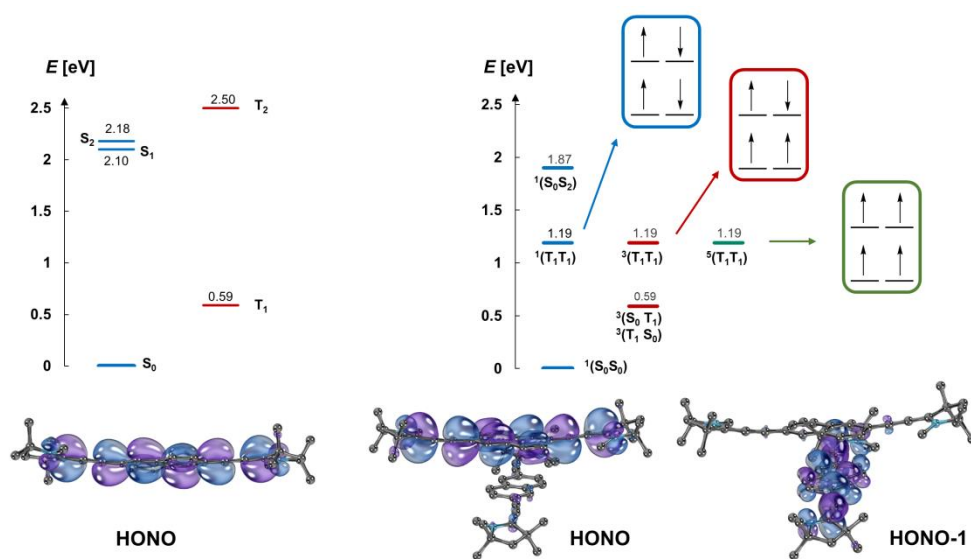


Figure S18: Electronic structure of 2^{monomer} (left) and 2^{dimer} as suggested by NEVPT2//sa-CASSCF(12,12) calculations.

Section S6. Configuration State Functions (CSFs)

2^{dimer}, sa-CASSCF(4,4) with eight singlet,
four triplet and one quintet roots.

Q₁	1.00000 [0]: 1111
T₁	0.80775 [1]: 2101 0.19022 [11]: 0121
T₂	0.75160 [3]: 1210 0.20122 [9]: 1012 0.04498 [6]: 1111
T₃	0.99389 [6]: 1111
T₄	0.98974 [0]: 2110 0.00645 [2]: 2011 0.00264 [6]: 1111
S₀	0.60663 [13]: 0220 0.15815 [18]: 0022 0.13955 [0]: 2200 0.04064 [5]: 2002 0.03672 [16]: 0121 0.00760 [2]: 2101 0.00446 [4]: 2011 0.00312 [7]: 1201
S₁	0.60848 [0]: 2200 0.16335 [5]: 2002 0.14326 [13]: 0220 0.03840 [18]: 0022 0.03653 [2]: 2101 0.00857 [16]: 0121
S₂	0.74800 [6]: 1210 0.19817 [12]: 1012 0.04484 [9]: 1111 0.00356 [4]: 2011
S₃	0.66263 [2]: 2101 0.15257 [16]: 0121 0.09243 [0]: 2200 0.04603 [5]: 2002 0.02369 [13]: 0220 0.01002 [18]: 0022 0.00548 [4]: 2011 0.00289 [8]: 1120
S₄	0.98797 [7]: 1201 0.00353 [0]: 2200
S₅	0.99085 [9]: 1111 0.00369 [1]: 2110
S₆	

0.98597 [1]: 2110
0.00661 [4]: 2011
0.00411 [9]: 1111

S₇	0.96891 [4]: 2011 0.00834 [8]: 1120 0.00714 [1]: 2110 0.00394 [0]: 2200 0.00278 [18]: 0022
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3^{dimer}, sa-CASSCF(4,4) with eight singlet,
four triplet and one quintet roots.

Q₁	1.00000 [0]: 1111
T₁	0.60825 [1]: 2101 0.33117 [11]: 0121 0.04810 [6]: 1111 0.00580 [8]: 1021 0.00580 [4]: 1201
T₂	0.46938 [3]: 1210 0.33174 [9]: 1012 0.18407 [6]: 1111 0.00868 [0]: 2110 0.00293 [12]: 0112
T₃	0.97266 [6]: 1111 0.01738 [2]: 2011 0.00965 [10]: 0211
T₄	0.90527 [0]: 2110 0.06945 [2]: 2011 0.01374 [5]: 1120 0.00785 [3]: 1210
S₀	0.26089 [13]: 0220 0.17411 [18]: 0022 0.10749 [6]: 1210 0.08996 [16]: 0121 0.07864 [0]: 2200 0.07201 [12]: 1012 0.05549 [7]: 1201 0.04503 [5]: 2002 0.04240 [9]: 1111 0.04049 [2]: 2101 0.01412 [11]: 1021 0.01022 [8]: 1120 0.00619 [10]: 1102
S₁	0.29336 [0]: 2200 0.20252 [5]: 2002 0.15566 [13]: 0220 0.11298 [2]: 2101

0,11270 [18]: 0022
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 0,00335 [5]: 2002

2^{dimer}, sa-CASSCF(8,8) with eight singlet, three triplet and one quintet roots.

Q₁

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T₁

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S₃

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3^{dimer}, sa-CASSCF(8,8) with eight singlet, three triplet and one quintet roots.

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2^{dimer}, sa-CASSCF(8,8) with twenty singlet, three triplet and one quintet roots.

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T₁

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2^{dimer}, sa-CASSCF(12,12) with four
 singlet, two triplet and two quintet roots.

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3_{dimer}, sa-CASSCF(12,12) with four
 singlet, two triplet and two quintet roots.

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Section S7. Diabatic Electronic States

The diabatic representation of states was calculated in order to obtain their electronic coupling. Particular attention was given to the singlet ground state ($^1|S_0S_0\rangle$), the triplet pair states ($^1|T_1T_1\rangle$), the initially excited singlet states ($^1|S_0S_1\rangle$ and $^1|S_1S_0\rangle$), the further locally excited singlet states ($^1|LE\rangle$), the charge transfer anion–cation ($^1|AC\rangle$) and cation–anion ($^1|CA\rangle$) singlet states and the doubly excited singlet states ($^1|DE\rangle$).

The diabatic wavefunctions (ϕ) are represented as a linear combination of adiabatic wavefunctions (ψ_i) where the expansion coefficients (C_i) are the configuration state function (CSF) coefficients as obtained from the sa-CASSCF calculations.

$$\Phi_i = \sum_i C_i \psi_i \quad \text{Eq.1}$$

The completeness of an adiabatic state (Σ) is the sum of the CSF coefficients used for the construction of the diabatic representation. Based on this definition an adiabatic state is well represented when Σ approaches unity. Note that for some adiabatic states, the Σ was moderate due to high multireference character. The active space of 4e/4o with eight singlet roots provides an excellent completeness, however the energetic ordering of the states is unsatisfactory in reference with the experiment (Table S1). The active space of 8e/8o with eight singlet roots provides a reasonable ordering of the electronic states; unfortunately with insufficient completeness (Table S2). The active space of 8e/8o with twenty singlet roots provides better energetic ordering and as well an improved completeness (Table S3). Increasing the active space to 12e/12o increases the completeness further (Table S4); unfortunately, at tremendous computational cost of the NEVPT2 calculation.

Table S1: Completeness and energies obtained by NEVPT2//sa-CASSCF(4,4) calculation with eight singlet, four triplet and one quintet roots.

Adiabatic state	2^{dimer}			3^{dimer}		
	Σ	E_{NEVPT2} [eV]	E_{CASSCF} [eV]	Σ	E_{NEVPT2} [eV]	E_{CASSCF} [eV]
S₀	0.96	0.00	5.66	0.77	0.0	5.81
S₁	0.99	0.88	0.0	0.80	1.35	0.0
S₂	0.80	0.99	5.00	0.70	1.36	5.78
S₃	0.84	1.01	5.14	0.99	1.56	0.14
S₄	0.99	1.87	4.40	0.76	1.84	5.47
S₅	0.99	1.95	1.05	0.94	2.35	5.44
S₆	1.00	2.15	3.95	1.00	2.65	4.58
S₇	0.98	3.00	5.50	0.89	3.02	5.59

Table S2: Completeness and energies obtained by NEVPT2//sa-CASSCF(8,8) calculation with eight singlet, three triplet and one quintet roots.

Adiabatic state	2^{dimer}			3^{dimer}		
	Σ	E_{NEVPT2} [eV]	E_{CASSCF} [eV]	Σ	E_{NEVPT2} [eV]	E_{CASSCF} [eV]
S₀	0.81	0.0	0.0	0.76	0.0	0.0
S₁	0.86	1.14	0.82	0.81	0.79	0.82
S₂	0.58	1.74	3.42	0.12	1.59	2.21
S₃	0.56	1.87	3.43	0.17	1.64	2.25
S₄	0.15	1.95	2.21	0.16	1.88	2.98
S₅	0.10	1.96	2.25	0.15	1.92	3.01
S₆	0.17	2.54	2.98	0.25	1.98	3.42
S₇	0.09	2.76	3.01	0.27	2.01	3.43

Table S3: Completeness and energies obtained by NEVPT2//sa-CASSCF(8,8) calculation with twenty singlet, three triplet and one quintet roots.

Adiabatic state	2^{dimer}			3^{dimer}		
	Σ	E_{NEVPT2} [eV]	E_{CASSCF} [eV]	Σ	E_{NEVPT2} [eV]	E_{CASSCF} [eV]
S₀	0.81	0.00	0.00	0.70	0.00	0.0
S₁	0.86	1.11	1.26	0.90	0.77	0.82
S₂	0.52	1.58	4.00	0.29	1.57	2.21
S₃	0.51	1.59	4.02	0.40	1.62	3.65
S₄	0.57	1.77	3.69	0.36	1.62	2.24
S₅	0.54	1.90	3.74	0.40	1.63	3.64
S₆	0.28	1.93	2.50	0.30	1.84	2.96
S₇	0.23	1.94	2.52	0.25	1.92	3.00
S₈	0.29	2.49	3.47	0.36	1.96	3.41
S₉	0.46	2.62	4.97	0.32	2.07	3.39
S₁₀	0.38	2.63	4.91	0.36	2.25	4.25
S₁₁	0.20	2.71	3.52	0.48	2.31	4.14
S₁₂	0.21	2.83	4.86	0.38	2.68	4.48
S₁₃	0.32	2.87	4.95	0.35	2.72	4.44
S₁₄	0.15	3.47	5.06	0.21	2.88	3.88

Table S4: Completeness and energies obtained by NEVPT2//sa-CASSCF(12,12) calculation with four singlet, three triplet and two quintet roots.

Adiabatic state	2^{dimer}			3^{dimer}		
	Σ	E_{NEVPT2} [eV]	E_{CASSCF} [eV]	Σ	E_{NEVPT2} [eV]	E_{CASSCF} [eV]
S₀	0.87	0.00	0.00	0.84	0.00	0.00
S₁	0.79	1.19	1.05	0.35	0.78	0.78
S₂	0.73	1.87	2.50	0.47	1.62	2.11
S₃	0.68	1.92	2.57	0.64	1.64	2.17

The selected expansion coefficients were orthogonalized by the Gram-Schmidt procedure.

Electronic couplings were calculated via the explicit construction of orthogonal diabatic states expressed as linear combinations of adiabats.²⁴⁻²⁶ Then the electronic couplings (V_{ij}) were calculated as follows:²⁷⁻²⁹

$$V_{ij} = \langle \Phi_i | H | \Phi_j \rangle = \sum_{a,b} C_{ia} C_{jb} \langle \psi_i | H | \psi_j \rangle = \sum_a C_{ia} C_{ja} \varepsilon_a \quad \text{Eq.2}$$

ε_a are the energies of the adiabatic states obtained from the NEVPT2//sa-CASSCF calculations.

For the **direct mechanism** the electronic coupling between $|^1(T_1T_1)\rangle$ and $|^1(S_1S_0)\rangle$ (or $|^1(T_1T_1)\rangle$ and $|^1(S_0S_1)\rangle$, respectively) was considered. Alternatively charge-transfer states could overall mediate the formation of $|^1(T_1T_1)\rangle$ (**mediated mechanism**) according to Eq. 3.

$$V_{eff} = V_{(S_1S_0)(T_1T_1)} - 2 \frac{V_{(S_1S_0)(CA)}V_{(CA)(T_1T_1)} + V_{(S_1S_0)(AC)}V_{(AC)(T_1T_1)}}{[(E_{CT} - E_{T_1T_1}) + (E_{CT} - E_{S_1S_0})]} \quad \text{Eq.3}$$

}
}

direct
mediated

Table S5: Orthogonalized CSF coefficients for 2^{dimer} obtained by NEVPT2//sa-CASSCF(8,8) calculation with twenty singlet, three triplet and one quintet roots at the TZVPP level of theory.

	$ ^1(S_0S_0)\rangle$	$ ^1(T_1T_1)\rangle$	$ ^1(DE)\rangle$	$ ^1(DE)\rangle$	$ ^1(DE)\rangle$	$ ^1(DE)\rangle$	$ ^1(S_1S_0)\rangle$	$ ^1(S_0S_1)\rangle$	$ ^1(AC)\rangle$	$ ^1(CA)\rangle$	$ ^1(AC)\rangle$	$ ^1(CA)\rangle$	$ ^1(CA)\rangle$	$ ^1(AC)\rangle$	$ ^1(AC)\rangle$
S ₀	1.00	-0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.02	-0.02	0.00	0.00	0.00
S ₁	0.00	0.95	0.02	0.05	0.00	0.00	0.00	0.00	0.00	-0.08	-0.23	-0.20	0.02	-0.01	0.02
S ₂	0.00	0.00	0.00	0.00	0.00	0.00	0.75	-0.65	-0.14	0.01	-0.03	0.03	0.00	-0.04	0.02
S ₃	0.00	0.00	0.00	0.00	0.00	0.00	0.03	-0.09	0.67	0.06	-0.14	0.16	-0.28	0.16	0.63
S ₄	0.00	0.00	0.00	0.00	0.00	0.00	0.65	0.75	0.02	0.01	-0.02	0.02	-0.07	-0.10	0.03
S ₅	0.00	0.00	0.00	0.00	0.00	0.00	0.09	-0.08	0.71	-0.10	0.24	-0.27	0.06	-0.17	-0.56
S ₆	0.02	0.25	-0.06	-0.21	-0.01	-0.36	0.00	0.00	0.00	-0.07	0.33	0.69	-0.28	0.18	-0.26
S ₇	0.02	0.18	-0.26	0.03	-0.15	0.42	0.00	0.00	0.00	0.11	0.66	0.12	0.32	-0.21	0.30
S ₈	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.02	0.19	0.17	-0.42	0.48	0.72	-0.03	-0.11
S ₉	0.00	0.08	0.00	-0.10	0.52	-0.06	0.00	0.00	0.00	0.82	0.10	-0.12	-0.07	0.04	-0.06
S ₁₀	0.00	0.00	0.09	0.91	0.26	-0.21	0.00	0.00	0.00	-0.07	0.15	0.12	0.03	-0.02	0.03
S ₁₁	0.00	0.00	0.00	0.00	0.00	0.00	0.12	0.05	0.02	-0.08	0.19	-0.22	0.30	0.90	-0.01
S ₁₂	0.00	0.01	0.66	-0.26	0.14	-0.41	0.00	0.00	0.00	-0.15	0.27	-0.11	0.30	-0.19	0.28
S ₁₃	0.00	0.05	0.64	0.18	-0.51	0.32	0.00	0.00	0.00	0.34	0.02	0.12	-0.17	0.11	-0.16
S ₁₄	0.00	0.02	0.28	-0.10	0.60	0.62	0.00	0.00	0.00	-0.33	-0.03	0.21	-0.09	0.06	-0.08

Table S6: Orthogonalized CSF coefficients for 3^{dimer} obtained by NEVPT2//sa-CASSCF(8,8) calculation with twenty singlet, three triplet and one quintet roots at the TZVPP level of theory.

	$ ^1(S_0S_0)\rangle$	$ ^1(T_1T_1)\rangle$	$ ^1(DE)\rangle$	$ ^1(DE)\rangle$	$ ^1(DE)\rangle$	$ ^1(DE)\rangle$	$ ^1(S_1S_0)\rangle$	$ ^1(S_0S_1)\rangle$	$ ^1(AC)\rangle$	$ ^1(CA)\rangle$	$ ^1(AC)\rangle$	$ ^1(CA)\rangle$	$ ^1(LE)\rangle$	$ ^1(DE)\rangle$	$ ^1(AC)\rangle$
S ₀	1.00	0.00	0.00	-0.04	0.05	-0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S ₁	0.00	0.67	0.03	-0.01	0.09	0.10	-0.01	0.00	0.00	0.00	0.71	-0.15	-0.02	-0.02	0.00
S ₂	0.00	0.00	0.29	0.14	0.51	0.42	-0.03	0.00	-0.01	0.01	0.01	0.66	0.17	0.01	0.00
S ₃	0.00	0.00	0.00	0.00	0.00	0.00	0.81	0.01	-0.48	-0.15	0.00	-0.03	0.24	-0.21	-0.02
S ₄	0.07	0.01	0.03	0.52	-0.65	0.55	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00
S ₅	0.00	0.00	0.00	0.00	0.00	0.00	0.21	0.07	0.00	0.96	0.00	0.01	-0.07	0.05	0.13
S ₆	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.64	0.01	0.05	0.00	0.00	-0.02	0.01	-0.77
S ₇	0.00	0.00	0.00	0.00	0.06	0.07	0.42	-0.04	0.18	-0.16	0.00	0.09	-0.64	0.58	-0.01

S ₈	0.00	0.00	0.00	0.00	0.00	0.00	0.36	-0.02	0.86	-0.04	0.00	-0.03	0.27	-0.24	-0.02
S ₉	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.77	0.03	-0.14	-0.01	0.00	0.00	0.01	0.62
S ₁₀	0.00	0.00	0.20	0.79	0.36	-0.32	0.00	0.00	0.00	0.00	-0.06	-0.31	-0.06	-0.02	0.00
S ₁₁	0.00	0.00	0.94	-0.23	-0.21	-0.08	0.01	0.00	0.00	0.00	-0.04	-0.13	-0.03	0.01	0.00
S ₁₂	0.00	0.27	0.00	0.16	-0.36	-0.60	0.03	-0.01	0.01	-0.01	0.01	0.63	0.00	0.00	0.00
S ₁₃	0.00	0.66	-0.03	-0.06	0.08	0.15	-0.01	-0.01	0.00	0.00	-0.68	-0.07	-0.16	-0.18	0.00
S ₁₄	0.00	0.19	-0.01	0.00	-0.02	-0.03	0.00	0.00	0.00	0.01	-0.15	-0.13	0.64	0.72	-0.01

Table S7: Energies and coupling matrix elements of the low-lying diabatic electronic states of 2^{dimer} calculated at the NEVPT2//sa-CASSCF(8,8) with twenty singlet, three triplet and one quintet roots level of theory. The electronic coupling V for the direct mechanism is highlighted in yellow, and those for the mediated mechanism are highlighted in green and orange.

V_{ij}	$ ^1(S_0S_0)\rangle$	$ ^1(T_1T_1)\rangle$	$ ^1(DE)\rangle$	$ ^1(DE)\rangle$	$ ^1(DE)\rangle$	$ ^1(DE)\rangle$	$ ^1(S_1S_0)\rangle$	$ ^1(S_0S_1)\rangle$	$ ^1(AC)\rangle$	$ ^1(CA)\rangle$	$ ^1(AC)\rangle$	$ ^1(CA)\rangle$	$ ^1(CA)\rangle$	$ ^1(AC)\rangle$	$ ^1(AC)\rangle$
$ ^1(S_0S_0)\rangle$	1	16	-10	-8	-5	-3	0	0	0	0	34	33	-3	2	-2
$ ^1(T_1T_1)\rangle$	16	1205	32	-45	22	26	0	0	0	107	185	159	-26	16	-24
$ ^1(DE)\rangle$	-10	32	2829	-36	54	203	0	0	0	-26	172	109	40	-26	38
$ ^1(DE)\rangle$	-8	-45	-36	2627	-76	-77	0	0	0	45	46	109	-64	41	-60
$ ^1(DE)\rangle$	-5	22	54	-76	2981	305	0	0	0	-204	63	106	18	-12	17
$ ^1(DE)\rangle$	-3	26	203	-77	305	2801	0	0	0	-182	-142	265	-244	157	-227
$ ^1(S_1S_0)\rangle$	0	0	0	0	0	0	1682	98	29	-9	23	-26	45	102	-15
$ ^1(S_0S_1)\rangle$	0	0	0	0	0	0	98	1697	-11	2	-4	5	19	43	16
$ ^1(AC)\rangle$	0	0	0	0	0	0	29	-11	1782	7	-17	19	144	-23	-142
$ ^1(CA)\rangle$	0	107	-26	45	-204	-182	-9	2	7	2714	-26	-85	-31	-4	-106
$ ^1(AC)\rangle$	34	185	172	46	63	-142	23	-4	-17	-26	2100	-201	-62	99	129
$ ^1(CA)\rangle$	33	159	109	109	106	265	-26	5	19	-85	-201	2159	92	-126	-124
$ ^1(CA)\rangle$	-3	-26	40	-64	18	-244	45	19	144	-31	-62	92	2381	133	132
$ ^1(AC)\rangle$	2	16	-26	41	-12	157	102	43	-23	-4	99	-126	133	2602	-111
$ ^1(AC)\rangle$	-2	-24	38	-60	17	-227	-15	16	-142	-106	129	-124	132	-111	1900

In the 2^{dimer} , no direct coupling between $|^1(T_1T_1)\rangle$ and $|^1(S_1S_0)\rangle$ (or $|^1(T_1T_1)\rangle$ and $|^1(S_0S_1)\rangle$) was obtained (Figure S7, yellow). Instead, a mediated mechanism based on coupling between the $|^1(S_1S_0)\rangle$ and $|^1(S_0S_1)\rangle$ states with the $|^1(AC)\rangle$ and $|^1(CA)\rangle$ states (Table S7, green), which in turn couple with the $|^1(T_1T_1)\rangle$ state, was predicted (Table S7, green). Overall, this leads to $V_{\text{eff}}=3$ meV.

Table S8: Energies and coupling matrix elements of the low-lying diabatic electronic states of $\mathbf{3}^{\text{dimer}}$ calculated at the NEVPT2//sa-CASSCF(8,8) with twenty singlet, three triplet and one quintet roots level of theory. The electronic coupling V for the direct mechanism is highlighted in yellow, and those for the mediated mechanism are highlighted in green and orange.

V_{ij}	$ ^1(S_0S_0)\rangle$	$ ^1(T_1T_1)\rangle$	$ ^1(DE)\rangle$	$ ^1(DE)\rangle$	$ ^1(DE)\rangle$	$ ^1(DE)\rangle$	$ ^1(S_1S_0)\rangle$	$ ^1(S_0S_1)\rangle$	$ ^1(AC)\rangle$	$ ^1(CA)\rangle$	$ ^1(AC)\rangle$	$ ^1(CA)\rangle$	$ ^1(LE)\rangle$	$ ^1(AC)\rangle$	$ ^1(DE)\rangle$
$ ^1(S_0S_0)\rangle$	9	1	4	62	-77	66	0	0	0	0	1	2	1	0	0
$ ^1(T_1T_1)\rangle$	1	1841	-42	9	-103	-129	7	-9	3	-4	-939	185	49	53	-4
$ ^1(DE)\rangle$	4	-42	2243	-48	-101	-102	6	0	3	-2	-27	-126	-37	-4	0
$ ^1(DE)\rangle$	62	9	-48	2081	142	-267	5	0	2	-2	32	-24	-11	6	0
$ ^1(DE)\rangle$	-77	-103	-101	142	1860	172	-4	0	-1	1	-118	-299	-57	-29	1
$ ^1(DE)\rangle$	66	-129	-102	-267	172	2087	-9	1	-4	3	-156	-340	-57	-41	2
$ ^1(S_1S_0)\rangle$	0	7	6	5	-4	-9	1716	-8	130	-23	8	25	-47	48	-4
$ ^1(S_0S_1)\rangle$	0	-9	0	0	0	1	-8	1972	4	-39	1	-2	0	0	110
$ ^1(AC)\rangle$	0	3	3	2	-1	-4	130	4	1883	-23	3	1	45	-39	1
$ ^1(CA)\rangle$	0	-4	-2	-2	1	3	-23	-39	-23	1650	-4	-13	35	-14	-46
$ ^1(AC)\rangle$	1	-939	-27	32	-118	-156	8	1	3	-4	1740	188	16	15	2
$ ^1(CA)\rangle$	2	185	-126	-24	-299	-340	25	-2	1	-13	188	2107	-99	-87	-1
$ ^1(LE)\rangle$	1	49	-37	-11	-57	-57	-47	0	45	35	16	-99	2304	473	-3
$ ^1(AC)\rangle$	0	53	-4	6	-29	-41	48	0	-39	-14	15	-87	473	2429	-6
$ ^1(DE)\rangle$	0	-4	0	0	1	2	-4	110	1	-46	2	-1	-3	-6	1923

In the $\mathbf{3}^{\text{dimer}}$, weak direct coupling between $|^1(T_1T_1)\rangle$ and $|^1(S_1S_0)\rangle$ (or $|^1(T_1T_1)\rangle$ and $|^1(S_0S_1)\rangle$) was obtained (Figure S8, yellow). Furthermore, a mediated mechanism including coupling between the $|^1(S_1S_0)\rangle$ and $|^1(S_0S_1)\rangle$ states with the $|^1(AC)\rangle$ and $|^1(CA)\rangle$ states (Table S7, green), which in turn couple with the $|^1(T_1T_1)\rangle$ state was predicted (Table S7, green). Overall, this leads to $V_{\text{eff}} = 17$ meV.

Table S9: Spin-orbit coupling matrix elements (in cm^{-1}) obtained from sa-CASSCF(12,12) calculation with four singlet, three triplet and two quintet roots via quasi-degenerate perturbation theory (QDPT) with the NEVPT2 diagonal energies.

2 ^{dimer}						3 ^{dimer}							
I(Mult.)	J(Mult.)	I	J	$\langle [L_x S] J \rangle$	$\langle [L_y S] J \rangle$	$\langle [L_z S] J \rangle$	I(Mult.)	J(Mult.)	I	J	$\langle [L_x S] J \rangle$	$\langle [L_y S] J \rangle$	$\langle [L_z S] J \rangle$
0(5)	0(5)	0	0	0.00	0.00	0.00	0(5)	0(5)	0	0	0.00	0.00	0.00
0(5)	0(5)	1	0	0.08	-0.01	-0.06	0(5)	0(5)	1	0	-0.30	0.00	0.34
0(5)	0(5)	1	1	0.00	0.00	0.00	0(5)	0(5)	1	1	0.00	0.00	0.00
0(5)	1(3)	0	0	-0.06	0.04	0.06	0(5)	1(3)	0	0	0.07	0.00	-0.08
0(5)	1(3)	0	1	0.00	-0.15	-0.01	0(5)	1(3)	0	1	0.00	-0.08	0.01
0(5)	1(3)	0	2	0.00	0.00	0.00	0(5)	1(3)	0	2	0.00	0.00	0.00
0(5)	1(3)	0	3	0.00	0.00	0.00	0(5)	1(3)	0	3	-0.24	-0.01	0.28
0(5)	1(3)	1	0	-0.29	0.08	0.27	0(5)	1(3)	1	0	0.14	-0.04	-0.16
0(5)	1(3)	1	1	-0.01	0.00	0.01	0(5)	1(3)	1	1	-0.01	0.00	0.01
0(5)	1(3)	1	2	-0.04	0.00	0.03	0(5)	1(3)	1	2	0.14	0.00	-0.16
0(5)	1(3)	1	3	0.00	-0.15	-0.01	0(5)	1(3)	1	3	-0.04	0.01	0.04
0(5)	2(1)	0	0	0.00	0.00	0.00	0(5)	2(1)	0	0	0.00	0.00	0.00
0(5)	2(1)	0	1	0.00	0.00	0.00	0(5)	2(1)	0	1	0.00	0.00	0.00
0(5)	2(1)	0	2	0.00	0.00	0.00	0(5)	2(1)	0	2	0.00	0.00	0.00
0(5)	2(1)	0	3	0.00	0.00	0.00	0(5)	2(1)	0	3	0.00	0.00	0.00
0(5)	2(1)	1	0	0.00	0.00	0.00	0(5)	2(1)	1	0	0.00	0.00	0.00
0(5)	2(1)	1	1	0.00	0.00	0.00	0(5)	2(1)	1	1	0.00	0.00	0.00
0(5)	2(1)	1	2	0.00	0.00	0.00	0(5)	2(1)	1	2	0.00	0.00	0.00
0(5)	2(1)	1	3	0.00	0.00	0.00	0(5)	2(1)	1	3	0.00	0.00	0.00
1(3)	1(3)	0	0	0.00	0.00	0.00	1(3)	1(3)	0	0	0.00	0.00	0.00
1(3)	1(3)	1	0	0.00	0.00	0.00	1(3)	1(3)	1	0	0.00	0.00	0.00
1(3)	1(3)	1	1	0.00	0.00	0.00	1(3)	1(3)	1	1	0.00	0.00	0.00
1(3)	1(3)	2	0	-0.06	0.03	0.06	1(3)	1(3)	2	0	0.06	0.00	-0.07
1(3)	1(3)	2	1	-0.01	0.15	0.02	1(3)	1(3)	2	1	-0.01	0.07	-0.01
1(3)	1(3)	2	2	0.00	0.00	0.00	1(3)	1(3)	2	2	0.00	0.00	0.00
1(3)	1(3)	3	0	0.00	-0.01	0.00	1(3)	1(3)	3	0	0.01	0.00	-0.01
1(3)	1(3)	3	1	0.08	-0.01	-0.06	1(3)	1(3)	3	1	0.01	0.00	-0.01
1(3)	1(3)	3	2	0.00	0.00	0.00	1(3)	1(3)	3	2	0.21	0.00	-0.24
1(3)	1(3)	3	3	0.00	0.00	0.00	1(3)	1(3)	3	3	0.00	0.00	0.00
1(3)	2(1)	0	0	-0.01	0.15	0.02	1(3)	2(1)	0	0	0.00	0.07	-0.01
1(3)	2(1)	0	1	-0.04	0.02	0.03	1(3)	2(1)	0	1	0.04	0.00	-0.04
1(3)	2(1)	0	2	0.00	-0.01	0.00	1(3)	2(1)	0	2	0.00	-0.12	0.02
1(3)	2(1)	0	3	0.03	-0.34	-0.06	1(3)	2(1)	0	3	-0.02	0.25	-0.03
1(3)	2(1)	1	0	0.06	-0.03	-0.06	1(3)	2(1)	1	0	-0.06	0.00	0.07
1(3)	2(1)	1	1	0.00	-0.08	-0.01	1(3)	2(1)	1	1	0.00	-0.03	0.01
1(3)	2(1)	1	2	-0.13	0.05	0.11	1(3)	2(1)	1	2	-0.20	0.00	0.22
1(3)	2(1)	1	3	0.01	-0.01	-0.01	1(3)	2(1)	1	3	-0.08	-0.01	0.09
1(3)	2(1)	2	0	0.00	0.00	0.00	1(3)	2(1)	2	0	0.00	0.01	0.00
1(3)	2(1)	2	1	0.00	0.00	0.00	1(3)	2(1)	2	1	0.00	0.00	0.00
1(3)	2(1)	2	2	0.00	0.00	0.00	1(3)	2(1)	2	2	0.00	0.00	0.00
1(3)	2(1)	2	3	0.00	0.00	0.00	1(3)	2(1)	2	3	-0.01	0.03	0.00

1(3)	2(1)	3 0	0.29	-0.08	-0.27	1(3)	2(1)	3 0	0.01	0.02	-0.01
1(3)	2(1)	3 1	0.00	0.00	0.00	1(3)	2(1)	3 1	-0.11	0.00	0.13
1(3)	2(1)	3 2	-0.07	0.01	0.06	1(3)	2(1)	3 2	0.00	-0.06	0.01
1(3)	2(1)	3 3	0.00	0.00	0.00	1(3)	2(1)	3 3	0.00	0.02	0.00

Section S8. XYZ Coordinates

1 monomer

N	-0.41120	-6.42400	-12.27530
N	-7.31540	-2.29070	-3.29580
C	-4.51780	-5.46380	-7.35300
C	-3.57630	-5.55860	-8.34020
C	-2.95010	-4.40340	-8.90020
C	-2.04690	-4.53790	-9.92550
C	-1.32040	-4.69650	-10.89600
C	3.35220	-2.64100	-11.97780
C	1.84640	-3.26140	-10.14830
C	2.09150	-3.42800	-11.64670
C	-2.96010	-2.04910	-14.40230
C	0.90270	-3.02770	-12.55910
C	0.05570	-1.87170	-11.99610
C	-1.00330	-1.39500	-12.97260
C	-1.90570	-2.50660	-13.38160
C	-1.10000	-3.65880	-13.95380
C	1.51240	-7.62470	-13.27780
C	-0.50420	-7.22660	-14.64040
C	2.16930	-8.41470	-9.82480
C	0.90310	-6.63290	-8.55540
C	1.07820	-7.33950	-9.88590
C	-3.85820	-8.23530	-13.62420
C	-4.29410	-6.35020	-12.05410
C	-3.21340	-7.19550	-12.71940
C	-0.25030	-7.91680	-10.35280
C	-0.83630	-8.92080	-9.58380
C	-2.09650	-9.37080	-9.84010
C	-2.82280	-8.84270	-10.85170
C	-2.31900	-7.84110	-11.67720
C	-0.98910	-7.43460	-11.44830
C	0.05150	-4.21300	-13.03980
C	0.87060	-5.23780	-13.83170
C	0.37220	-6.65210	-13.52190
C	-0.55820	-5.09490	-11.97020
C	-3.34890	-3.14980	-8.36770
C	-4.26590	-3.03690	-7.38350
C	-4.86800	-4.18510	-6.83730
C	-5.77840	-4.08490	-5.80580
C	-6.53350	-3.91680	-4.79110
C	-5.77640	-6.67830	-0.63020
C	-4.75530	-5.81470	-2.66260
C	-5.91860	-5.66080	-1.79590
C	-10.76000	-6.05110	-5.20160
C	-7.33300	-5.82030	-2.42760
C	-7.32470	-6.83180	-3.56590
C	-8.72100	-7.06420	-4.15330
C	-9.36890	-5.78710	-4.62330
C	-9.39630	-4.82200	-3.46360
C	-8.04690	-4.50450	-2.78460
C	-7.26350	-1.38410	-0.96590
C	-9.33420	-1.26490	-2.26430
C	-3.87890	-0.36650	-1.99580
C	-3.50430	-2.26560	-3.61470
C	-4.55440	-1.37880	-2.89600
C	-10.05570	-0.41670	-5.76310
C	-8.70490	-2.11870	-7.00050
C	-8.86950	-1.39110	-5.64710
C	-5.49500	-0.76680	-3.90160
C	-5.01730	0.22790	-4.72860
C	-5.77280	0.74560	-5.75850
C	-7.01940	0.24210	-6.00420
C	-7.56300	-0.77210	-5.21840
C	-6.81170	-1.23050	-4.13500
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C	-8.06680	-2.10070	-2.03090
C	-7.21550	-3.59750	-3.68180
H	-4.92090	-6.77570	-0.47610
H	-9.32530	-3.70280	-1.60370
H	-4.93550	-6.24630	-7.01580
H	-3.33060	-6.41810	-8.66220
H	3.19900	-1.68890	-11.79930
H	4.09330	-2.96160	-11.42240
H	3.57480	-2.76390	-12.92380
H	1.03400	-3.74770	-9.89350
H	2.61020	-3.61920	-9.64940
H	1.73660	-2.30970	-9.93930
H	2.28690	-4.39400	-11.81300
H	-2.51500	-1.77060	-15.22930
H	-3.57180	-2.79090	-14.59460
H	-3.46580	-1.29550	-14.03310
H	1.32460	-2.65980	-13.38770
H	0.65190	-1.11480	-11.77030
H	-0.38510	-2.17070	-11.16150
H	-0.56270	-1.01720	-13.77520
H	-1.53750	-0.67620	-12.55150
H	-2.38400	-2.83570	-12.56680
H	-1.72110	-4.40270	-14.15670
H	-0.70180	-3.36410	-14.81130
H	1.14920	-8.49240	-13.00470
H	2.03110	-7.73320	-14.10330
H	2.09460	-7.27560	-12.57130
H	-1.24180	-6.60880	-14.82650
H	0.03480	-7.34540	-15.44910
H	-0.86620	-8.09310	-14.35810
H	1.89080	-9.12950	-9.21450
H	2.31160	-8.78660	-10.72050
H	3.00320	-8.01560	-9.50140
H	0.73520	-7.29530	-7.85350
H	1.71650	-6.12980	-8.34330
H	0.14280	-6.01650	-8.61030
H	1.36420	-6.65580	-10.55570
H	-4.41670	-8.83410	-13.08710
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H	-3.15910	-8.75540	-14.07280
H	-3.87360	-5.66190	-11.49720
H	-4.84410	-5.92080	-12.74380
H	-4.85920	-6.92290	-11.49560
H	-2.65050	-6.59420	-13.28700
H	-0.34550	-9.30100	-8.86360
H	-2.46790	-10.06190	-9.30300
H	-3.70340	-9.16410	-11.00280
H	1.82700	-5.16070	-13.58910
H	0.78210	-5.05820	-14.80210
H	-2.95420	-2.35940	-8.71710
H	-4.50720	-2.17760	-7.05850
H	-6.33590	-6.39530	0.12210
H	-6.06240	-7.56490	-0.93530
H	-3.93860	-5.65110	-2.14530
H	-4.73610	-6.72450	-3.02570
H	-4.80990	-5.17030	-3.39960
H	-5.87320	-4.74490	-1.39610
H	-10.70540	-6.76520	-5.86990
H	-11.36640	-6.32310	-4.48140
H	-11.09910	-5.23420	-5.62270
H	-7.89380	-6.23670	-1.71350
H	-6.72160	-6.50850	-4.28150
H	-6.96600	-7.69140	-3.23170
H	-9.29550	-7.48550	-3.46520
H	-8.65130	-7.69160	-4.91620
H	-8.79900	-5.39300	-5.34500

H	-9.78750	-3.97050	-3.78250	C	-4.54881	-3.13641	-5.42439
H	-10.00760	-5.18680	-2.77550	C	-2.91957	-4.39209	-0.80634
H	-7.01390	-0.49360	-1.28930	C	-2.31380	-4.57423	-3.23874
H	-7.80340	-1.29750	-0.15260	C	-3.33030	-4.01342	-2.23475
H	-6.45250	-1.89790	-0.76600	C	-8.72139	-5.48558	-4.26076
H	-9.91650	-1.72440	-2.90370	C	-4.81874	-4.41450	-2.49527
H	-9.81080	-1.14840	-1.41440	C	-4.96826	-5.72417	-3.28307
H	-9.08510	-0.38660	-2.62140	C	-6.42755	-6.15178	-3.40690
H	-4.55450	0.22240	-1.60060	C	-7.25307	-5.08083	-4.12179
H	-3.39510	-0.83430	-1.28320	C	-7.13279	-3.76522	-3.35382
H	-3.24760	0.16810	-2.52220	C	-5.69053	-3.25876	-3.07956
H	-2.94590	-1.70710	-4.19300	C	-4.97831	0.34229	-2.19688
H	-2.94050	-2.71010	-2.94640	C	-7.20087	-0.22952	-3.13565
H	-3.96310	-2.94120	-4.15480	C	-1.61688	0.78973	-3.38019
H	-5.09830	-1.97870	-2.30860	C	-1.31702	-1.28127	-4.80756
H	-9.84210	0.28080	-6.41920	C	-2.33112	-0.34858	-4.12263
H	-10.85250	-0.90550	-6.05600	C	-8.01631	0.36675	-6.61491
H	-10.22720	-0.00430	-4.89180	C	-6.86270	-1.60671	-7.69001
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H	-9.54220	-2.57180	-7.23090	C	-3.34801	0.15382	-5.13725
H	-8.48270	-1.46670	-7.69630	C	-2.92561	1.04587	-6.13145
H	-9.11330	-2.07990	-4.96350	C	-3.77115	1.40924	-7.17570
H	-4.14170	0.56770	-4.58360	C	-5.04905	0.86296	-7.25609
H	-5.42940	1.44970	-6.29710	C	-5.52454	-0.01638	-6.27508
H	-7.52750	0.59170	-6.72590	C	-4.67776	-0.33075	-5.18473
H	-7.79180	-3.78590	-0.85140	C	-5.76298	-2.07289	-2.07920

2monomer

N	2.87614	-6.44746	-14.54856	C	-5.77724	-0.76379	-2.89526
N	-5.13434	-1.21264	-4.15629	C	-5.08882	-2.58996	-4.30909
C	-1.33169	-5.75843	-9.99015	H	-1.87632	-4.10365	-0.59728
C	-0.45086	-5.70506	-11.02565	H	-6.63977	-2.15202	-1.42141
C	0.10138	-4.43941	-11.48268	H	-1.73539	-6.72121	-9.66591
C	1.02402	-4.45806	-12.49607	H	-0.13521	-6.61719	-11.53372
C	1.89765	-4.62517	-13.38069	H	7.06125	-2.63870	-12.77897
C	6.88478	-3.72674	-12.84016	H	7.35961	-4.18973	-11.95965
C	4.72521	-3.66976	-11.55401	H	7.40511	-4.09598	-13.73942
C	5.38254	-4.03165	-12.89239	H	3.64713	-3.87325	-11.55460
C	2.06958	-1.62275	-17.20087	H	5.17736	-4.26562	-10.74521
C	4.73786	-3.37013	-14.15413	H	4.87417	-2.60849	-11.29957
C	3.96937	-2.07827	-13.83746	H	5.27613	-5.12376	-12.99652
C	3.45552	-1.38290	-15.09475	H	2.92392	-1.35756	-17.84736
C	2.55645	-2.30473	-15.92200	H	1.40330	-2.28033	-17.78269
C	3.31372	-3.59125	-16.24744	H	1.51636	-0.69820	-16.97720
C	4.73588	-8.02802	-15.09609	H	5.57050	-3.07246	-14.81873
C	3.31754	-7.12267	-16.92047	H	4.62700	-1.39571	-13.27489
C	4.38053	-8.89598	-11.63269	H	3.11724	-2.30508	-13.17927
C	3.16051	-6.89235	-10.68398	H	4.30876	-1.06209	-15.72217
C	3.52825	-7.66269	-11.96390	H	2.90966	-0.46404	-14.82455
C	-0.26884	-7.58052	-16.93257	H	1.68220	-2.57627	-15.30366
C	-0.94264	-5.77209	-15.30189	H	2.66576	-4.26813	-16.82538
C	0.18496	-6.72037	-15.74476	H	4.15925	-3.33099	-16.91100
C	2.27476	-8.00934	-12.75446	H	4.09223	-8.91234	-14.97412
C	1.36244	-8.92326	-12.21125	H	5.49239	-8.26181	-15.86099
C	0.13906	-9.17013	-12.82804	H	5.25882	-7.84349	-14.14942
C	-0.20788	-8.47536	-13.98371	H	2.74218	-6.27950	-17.32324
C	0.67163	-7.55332	-14.56687	H	4.12345	-7.35588	-17.63367
C	1.94406	-7.36780	-13.97289	H	2.65421	-7.99732	-16.86230
C	3.90065	-4.35412	-15.03004	H	3.85323	-9.57512	-10.94352
C	4.77933	-5.52439	-15.55067	H	4.63751	-9.47112	-12.53473
C	3.92025	-6.80884	-15.53983	H	5.31881	-8.59358	-11.13973
C	2.81827	-5.09503	-14.25533	H	2.57146	-7.51979	-9.99596
C	-0.35000	-3.25103	-10.82623	H	4.07238	-6.57317	-10.15410
C	-1.26277	-3.29200	-9.78951	H	2.56561	-5.99857	-10.91319
C	-3.91499	-3.37228	-6.48192	H	4.13087	-6.98581	-12.58265

H	-1.14850	-8.19076	-16.67178
H	-0.55410	-6.94170	-17.78433
H	0.52242	-8.26653	-17.27004
H	-0.62945	-5.15761	-14.44739
H	-1.22863	-5.09734	-16.12582
H	-1.84328	-6.33471	-15.00683
H	1.02048	-6.09244	-16.07530
H	1.60073	-9.42816	-11.27249
H	-0.56456	-9.87514	-12.38799
H	-1.19285	-8.63633	-14.42806
H	5.64261	-5.67084	-14.88832
H	5.17606	-5.31293	-16.55350
H	0.00807	-2.28261	-11.17536
H	-3.56444	-3.90441	-0.05666
H	-2.99811	-5.48239	-0.65237
H	-1.31782	-4.14881	-3.03610
H	-2.22347	-5.66907	-3.15853
H	-2.57452	-4.32878	-4.27560
H	-3.26270	-2.91584	-2.31345
H	-8.82547	-6.45724	-4.76662
H	-9.19469	-5.57748	-3.26808
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H	-4.54011	-5.60821	-4.29109
H	-4.38425	-6.51455	-2.78380
H	-6.85630	-6.32261	-2.40115
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H	-6.82541	-4.93475	-5.13108
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H	-7.62241	-3.90660	-2.37270
H	-4.88924	1.23265	-2.83729
H	-5.49933	0.63896	-1.27350
H	-3.97014	0.00792	-1.92278
H	-7.85118	-0.97540	-3.60880
H	-7.65743	0.05951	-2.17631
H	-7.17363	0.66142	-3.77909
H	-2.32954	1.47979	-2.90351
H	-0.95744	0.38208	-2.59685
H	-0.98493	1.38226	-4.06137
H	-0.73249	-0.74308	-5.57118
H	-0.61203	-1.69261	-4.06671
H	-1.82103	-2.12067	-5.30453
H	-2.87186	-0.95349	-3.38368
H	-7.89075	0.97698	-7.52402
H	-8.99226	-0.13987	-6.69215
H	-8.05489	1.05354	-5.75611
H	-6.04600	-2.33568	-7.60743
H	-7.81459	-2.15712	-7.77151
H	-6.72376	-1.04347	-8.62732
H	-7.09604	-1.28227	-5.59354
H	-1.90498	1.43370	-6.10722
H	-3.42235	2.08413	-7.95630
H	-5.68147	1.10548	-8.11059
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C	-1.75851	-2.09558	-9.15571
C	-1.77759	-4.56729	-9.30707
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C	-2.64426	-2.14691	-8.12636
C	-2.66091	-4.60926	-8.24348
H	-3.01081	-1.22910	-7.66864
H	-3.03565	-5.57271	-7.89923
C	-3.11193	-3.41599	-7.59332

3monomer

N	2.44973	-6.57061	-15.94689
N	-7.03043	-2.45516	-3.73110
C	-1.43407	-5.76576	-10.99756
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C	-0.11276	-4.55047	-12.65847
C	0.72353	-4.60635	-13.73857
C	1.48854	-4.79870	-14.70600
C	6.48926	-3.50404	-15.25965
C	4.70318	-3.88800	-13.53837
C	5.06748	-4.02541	-15.02169
C	0.43016	-1.81151	-18.01716
C	4.05725	-3.37205	-16.01693
C	3.30639	-2.17256	-15.41713
C	2.37602	-1.49530	-16.42214
C	1.36961	-2.48433	-17.01787
C	2.12587	-3.65413	-17.65087
C	4.53349	-7.77388	-16.56813
C	2.65714	-7.60661	-18.21145
C	4.57989	-8.55402	-13.05995
C	3.12318	-6.77283	-12.01906
C	3.50453	-7.49223	-13.32813
C	-0.85490	-8.15999	-17.82003
C	-1.44184	-6.32880	-16.17784
C	-0.31172	-7.20070	-16.75292
C	2.25337	-8.05922	-13.98965
C	1.53305	-9.05213	-13.31060
C	0.29969	-9.49897	-13.77765
C	-0.26255	-8.91320	-14.90977
C	0.41849	-7.91956	-15.62555
C	1.71572	-7.54633	-15.19560
C	3.09280	-4.39949	-16.68990
C	3.87772	-5.48179	-17.48640
C	3.37917	-6.88985	-17.05942
C	2.29938	-5.22729	-15.69891
C	-0.49245	-3.32770	-12.00879
C	-1.29122	-3.33849	-10.89774
C	-1.79318	-4.55299	-10.31390
C	-5.14545	-4.48814	-5.73672
C	-5.98071	-4.26609	-4.83582
C	-6.23291	-5.87017	0.10523
C	-4.62467	-5.49677	-1.78514
C	-6.05720	-5.25758	-1.29017
C	-9.66718	-6.84908	-5.74286
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C	-6.77047	-6.92475	-3.13648
C	-7.90913	-7.44375	-4.01416
C	-8.51523	-6.33564	-4.88118
C	-8.96174	-5.17975	-3.98429
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C	-7.43985	-1.22169	-1.60845
C	-9.23995	-1.36285	-3.33770
C	-3.87870	-0.64958	-1.81754
C	-3.11167	-2.51451	-3.33654
C	-4.31958	-1.68682	-2.85919
C	-9.05671	-0.69673	-6.87560
C	-7.58092	-2.60002	-7.63335
C	-8.01197	-1.73230	-6.43588
C	-5.02658	-1.06811	-4.05965
C	-4.34012	-0.11135	-4.82001
C	-4.86470	0.37137	-6.01629
C	-6.06493	-0.14348	-6.50049
C	-6.79233	-1.09807	-5.77638
C	-6.29367	-1.50766	-4.51441
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H	-9.54822	-3.59142	-2.11477
H	-1.81174	-6.71987	-10.63005
H	-0.38332	-6.71389	-12.60458
H	6.54714	-2.41739	-15.07281
H	7.21223	-3.99141	-14.58669
H	6.81806	-3.68574	-16.29653
H	3.67603	-4.21099	-13.32793
H	5.37833	-4.50693	-12.92705
H	4.81400	-2.84856	-13.19165
H	5.08316	-5.10586	-15.23691
H	0.99442	-1.36639	-18.85497
H	-0.29285	-2.52731	-18.44224
H	-0.14185	-1.00393	-17.53152
H	4.64966	-2.97684	-16.86339
H	4.04028	-1.44460	-15.03454
H	2.71268	-2.50190	-14.55220
H	2.96967	-1.05340	-17.24540
H	1.84326	-0.65935	-15.93750
H	0.75927	-2.88587	-16.19219
H	1.41292	-4.38054	-18.07796
H	2.72661	-3.27043	-18.49716
H	4.15620	-8.71901	-16.15130
H	5.20754	-8.01524	-17.40461
H	5.11993	-7.26295	-15.79323
H	1.86731	-6.97975	-18.64746
H	3.37904	-7.84656	-19.00633
H	2.20421	-8.54752	-17.86724
H	4.22416	-9.31823	-12.35065
H	4.88895	-9.06916	-13.98152
H	5.47161	-8.08344	-12.61378
H	2.66884	-7.47247	-11.29948
H	4.01584	-6.33513	-11.54450
H	2.40132	-5.96560	-12.20010
H	3.93216	-6.73962	-14.00289
H	-1.60941	-8.84465	-17.40040
H	-1.34150	-7.59650	-18.63244
H	-0.05576	-8.77318	-18.26264
H	-1.05964	-5.62334	-15.42691
H	-1.92814	-5.75147	-16.98186
H	-2.21449	-6.95003	-15.69676
H	0.40234	-6.52296	-17.23641
H	1.93775	-9.46335	-12.38363
H	-0.24499	-10.27502	-13.23384
H	-1.25792	-9.22030	-15.23677
H	4.95600	-5.39512	-17.29905
H	3.73103	-5.34056	-18.56641
H	-0.11595	-2.38473	-12.41297
H	-1.54745	-2.38195	-10.44275
H	-7.22168	-5.63098	0.53116
H	-6.14283	-6.96965	0.06464
H	-3.91156	-4.98365	-1.12103
H	-4.36608	-6.56765	-1.77406
H	-4.46465	-5.11782	-2.80277
H	-6.16740	-4.16628	-1.18125
H	-9.32348	-7.63629	-6.43350
H	-10.46880	-7.27803	-5.11702
H	-10.11137	-6.04090	-6.34731
H	-8.01460	-6.10815	-1.61086
H	-5.93429	-6.62234	-3.78275
H	-6.39252	-7.73786	-2.49516
H	-8.70833	-7.87105	-3.37903
H	-7.54676	-8.26667	-4.65319
H	-7.72730	-5.95909	-5.55463
H	-9.38930	-4.36837	-4.59743
H	-9.77582	-5.53512	-3.32446
H	-7.04459	-0.28271	-2.02346
H	-8.21055	-0.96810	-0.86460
H	-6.62341	-1.74255	-1.09087

H	-9.75765	-1.98574	-4.07936
H	-9.96489	-1.09227	-2.55522
H	-8.91028	-0.43648	-3.82987
H	-4.72987	-0.06862	-1.43309
H	-3.39146	-1.14943	-0.96428
H	-3.15002	0.06100	-2.23989
H	-2.35585	-1.87076	-3.81431
H	-2.63221	-3.02157	-2.48418
H	-3.41353	-3.27762	-4.06675
H	-5.01899	-2.38027	-2.37485
H	-8.65199	-0.01749	-7.64288
H	-9.93337	-1.19903	-7.31585
H	-9.40337	-0.08089	-6.03242
H	-6.85655	-3.36898	-7.33525
H	-8.45712	-3.10049	-8.07834
H	-7.11228	-1.98500	-8.41830
H	-8.48203	-2.40010	-5.70374
H	-3.36644	0.24396	-4.47703
H	-4.31483	1.11793	-6.59527
H	-6.43834	0.18786	-7.47142
H	-8.08595	-3.60858	-1.13148
C	-2.59518	-4.55433	-9.13519
C	-2.98241	-3.33895	-8.47203
C	-3.07248	-5.77004	-8.53319
H	-2.63750	-2.38110	-8.86102
H	-2.78539	-6.72757	-8.96772
C	-3.78051	-3.32960	-7.36276
C	-3.87531	-5.78040	-7.42444
H	-4.06798	-2.38817	-6.89079
H	-4.22858	-6.72484	-7.00302
C	-4.28553	-4.55551	-6.79789

Truncated 2^{monomer}

N	7.28844	0.52561	-4.36207
C	3.12254	0.31923	1.93740
H	4.19738	0.40657	2.11240
C	2.24575	0.32779	3.04912
N	-2.06853	0.13927	6.22616
C	0.40421	0.10187	1.48841
H	-0.52719	0.00936	0.92960
C	5.04987	0.36303	-3.52834
C	-0.74581	0.30735	5.99490
C	0.86863	0.19289	2.77381
C	0.01942	0.54193	7.28037
C	8.07243	0.59201	-5.64119
C	5.93719	0.43944	-4.56147
C	0.34921	0.20052	3.65998
C	5.11241	-1.09420	-6.37148
H	4.95921	-1.20114	-7.45726
H	5.85163	-1.84395	-6.04969
C	-0.18174	0.22875	4.74674
C	2.38099	0.17857	0.57414
C	4.20172	0.29823	-2.64023
C	3.42099	0.22381	-0.32046
H	4.44955	0.28929	0.04211
C	1.03017	0.09136	0.16086
C	6.98151	0.56239	-6.69667
H	7.18519	-0.21168	-7.44975
H	6.97690	1.51760	-7.24416
C	8.89171	1.86843	-5.70643
H	8.24457	2.75362	-5.59355
H	9.40591	1.94545	-6.67783
H	9.65884	1.90534	-4.91661
C	5.60178	0.34293	-6.03386
C	3.18295	0.20834	-1.70935

C	1.83463	0.11917	-2.13580	H	-1.65145	-1.79638	-8.97350
H	1.62631	0.10450	-3.20821	H	-0.07662	-2.43560	-8.42377
C	-2.44128	0.27049	7.68326	C	-0.84081	0.36398	6.10754
C	4.54757	1.36370	-6.57070	C	1.54010	0.00824	-1.25264
H	4.41651	1.21999	-7.65416	H	2.40654	0.05261	-0.59264
C	0.81135	0.07140	-1.24239	C	0.88080	-0.08627	-4.88829
H	-0.20529	0.01390	-1.63190	C	1.76619	-0.03500	-2.60579
C	9.02293	-0.59303	-5.78825	H	2.78924	-0.01231	-2.98859
H	9.79123	-0.60478	-4.99868	C	0.23678	-0.02052	-0.70159
H	9.54140	-0.54107	-6.75834	C	0.42097	-0.11870	-9.79128
H	8.47319	-1.54664	-5.74357	H	0.08050	-0.92920	-10.45081
C	-1.13414	0.79859	8.28314	H	0.08445	0.81508	-10.26771
H	-0.92814	0.33975	9.26163	C	2.54595	1.11675	-10.33285
H	-1.23133	1.88129	8.45467	H	2.13794	2.03915	-9.88809
C	0.99809	1.73699	7.26620	H	2.31980	1.13091	-11.41109
C	-3.55340	1.28692	7.87079	H	3.64148	1.14043	-10.21923
H	-3.29858	2.24281	7.38807	C	-0.21764	-0.23925	-8.38814
H	-3.71268	1.47488	8.94453	C	0.69342	-0.08742	-3.51811
H	-4.51014	0.93382	7.45242	C	-0.61644	-0.11875	-2.97864
C	0.75565	-0.73768	7.66808	H	-1.46363	-0.16061	-3.66725
C	-2.88643	-1.05865	8.26399	C	-1.99063	0.84752	9.59673
H	-3.77840	-1.44171	7.74254	C	-1.35182	0.81715	-8.19021
H	-3.14111	-0.94588	9.32954	H	-2.14919	0.64194	-8.92862
H	-2.09773	-1.82133	8.18089	C	-0.83051	-0.07897	-1.63693
H	1.43256	1.87796	8.26821	H	-1.86151	-0.09531	-1.28290
H	1.81765	1.56261	6.55162	C	2.54852	-1.34955	-10.32625
H	0.48097	2.66271	6.96999	H	3.64388	-1.37451	-10.21053
H	1.26107	-0.61524	8.64087	H	2.32602	-1.36058	-11.40466
H	0.06857	-1.59224	7.75049	H	2.13741	-2.26979	-9.88158
H	1.51941	-0.99595	6.91760	C	-0.52280	1.27754	9.68554
H	3.57603	1.21631	-6.07480	H	-0.03957	0.86981	10.58590
H	4.87977	2.39695	-6.38384	H	-0.47596	2.37386	9.76930
H	4.16205	-1.31577	-5.86140	C	1.21663	1.91481	7.94501
C	7.89221	0.55981	-3.02222	C	-2.89811	1.98492	10.03023
H	8.97347	0.38936	-3.10521	H	-2.74635	2.87269	9.39737
H	7.71283	1.52873	-2.52264	H	-2.67825	2.26360	11.07312
H	7.45171	-0.22917	-2.39235	H	-3.96310	1.70480	9.98133
C	-2.99533	-0.18148	5.13114	C	0.93547	-0.48667	8.65078
H	-4.02061	-0.22503	5.52132	C	-2.31705	-0.38381	10.42093
H	-2.94341	0.59301	4.34869	H	-3.35751	-0.70765	10.25712
H	-2.73771	-1.14830	4.66481	H	-2.19530	-0.17036	11.49451
H	2.61344	0.43253	4.05919	H	-1.66010	-1.22843	10.16465

Truncated 3^{monomer}

N	2.15147	-0.08821	-8.19430
C	0.82877	0.13545	3.02453
H	1.67096	0.22377	3.71480
C	-0.48449	0.08317	3.55119
N	-2.13237	0.57591	8.11841
C	0.00086	0.00006	0.72066
C	-1.29809	-0.08411	1.27342
H	-2.15989	-0.17828	0.61253
C	0.96414	-0.09938	-6.11515
C	1.06167	0.08986	1.66342
H	2.09567	0.14296	1.32227
C	-0.95217	0.58860	7.45638
C	-1.53740	-0.05053	2.62169
H	-2.56419	-0.11291	2.99065
C	0.21088	0.83215	8.39502
C	1.93511	-0.11029	-9.68020
C	0.98486	-0.10823	-7.47898
C	-0.70337	0.20413	4.91618
C	-0.83629	-1.65897	-8.24517

H	-1.65145	-1.79638	-8.97350
H	-0.07662	-2.43560	-8.42377
C	-0.84081	0.36398	6.10754
C	1.54010	0.00824	-1.25264
H	2.40654	0.05261	-0.59264
C	0.88080	-0.08627	-4.88829
C	1.76619	-0.03500	-2.60579
H	2.78924	-0.01231	-2.98859
C	0.23678	-0.02052	-0.70159
C	0.42097	-0.11870	-9.79128
H	0.08050	-0.92920	-10.45081
H	0.08445	0.81508	-10.26771
C	2.54595	1.11675	-10.33285
H	2.13794	2.03915	-9.88809
H	2.31980	1.13091	-11.41109
H	3.64148	1.14043	-10.21923
C	-0.21764	-0.23925	-8.38814
C	0.69342	-0.08742	-3.51811
C	-0.61644	-0.11875	-2.97864
H	-1.46363	-0.16061	-3.66725
C	-1.99063	0.84752	9.59673
C	-1.35182	0.81715	-8.19021
H	-2.14919	0.64194	-8.92862
C	-0.83051	-0.07897	-1.63693
H	-1.86151	-0.09531	-1.28290
C	2.54852	-1.34955	-10.32625
H	3.64388	-1.37451	-10.21053
H	2.32602	-1.36058	-11.40466
H	2.13741	-2.26979	-9.88158
C	-0.52280	1.27754	9.68554
H	-0.03957	0.86981	10.58590
H	-0.47596	2.37386	9.76930
C	1.21663	1.91481	7.94501
C	-2.89811	1.98492	10.03023
H	-2.74635	2.87269	9.39737
H	-2.67825	2.26360	11.07312
H	-3.96310	1.70480	9.98133
C	0.93547	-0.48667	8.65078
C	-2.31705	-0.38381	10.42093
H	-3.35751	-0.70765	10.25712
H	-2.19530	-0.17036	11.49451
H	-1.66010	-1.22843	10.16465
H	1.96767	2.07998	8.73324
H	1.73777	1.60613	7.02531
H	0.70181	2.86618	7.74017
H	1.74218	-0.34933	9.39046
H	0.25220	-1.25709	9.03647
H	1.38592	-0.87529	7.72379
H	-1.78268	0.74044	-7.18025
H	-0.95791	1.83695	-8.32331
H	-1.24317	-1.81034	-7.23324
C	3.47391	-0.03866	-7.55430
H	4.24760	-0.27025	-8.29783
H	3.67426	0.95585	-7.11685
H	3.52462	-0.77953	-6.74078
C	-3.39081	0.27710	7.41988
H	-4.22926	0.36816	8.12277
H	-3.54280	0.98493	6.58884
H	-3.37565	-0.74172	6.99521

2^{dimer, singlet}

N	2.87446	-6.44698	-14.54940
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N	-5.13654	-1.21585	-4.15691	H	7.05617	-2.63259	-12.78173
C	-1.32991	-5.75872	-9.98974	H	7.35644	-4.18280	-11.96158
C	-0.44917	-5.70476	-11.02526	H	7.40357	-4.08959	-13.74133
C	0.10203	-4.43873	-11.48246	H	3.64283	-3.87270	-11.56064
C	1.02369	-4.45690	-12.49677	H	5.17278	-4.26236	-10.74937
C	1.89668	-4.62394	-13.38204	H	4.86751	-2.60585	-11.30447
C	6.88168	-3.72096	-12.84273	H	5.27565	-5.12087	-13.00025
C	4.72059	-3.66741	-11.55882	H	2.91961	-1.36152	-17.85464
C	5.38002	-4.02853	-12.89637	H	1.39909	-2.28433	-17.78767
C	2.06567	-1.62583	-17.20724	H	1.51251	-0.70098	-16.98460
C	4.73539	-3.36863	-14.15896	H	5.56801	-3.07184	-14.82398
C	3.96687	-2.07634	-13.84401	H	4.62456	-1.39299	-13.28248
C	3.45302	-1.38289	-15.10236	H	3.11477	-2.30216	-13.18542
C	2.55330	-2.30582	-15.92761	H	4.30635	-1.06395	-15.73064
C	3.31037	-3.59284	-16.25151	H	2.90813	-0.46294	-14.83389
C	4.73422	-8.02778	-15.09623	H	1.67934	-2.57632	-15.30842
C	3.31513	-7.12415	-16.92091	H	2.66204	-4.27062	-16.82798
C	4.38453	-8.88937	-11.63290	H	4.15543	-3.33351	-16.91604
C	3.16176	-6.88782	-10.68340	H	4.09070	-8.91202	-14.97305
C	3.52961	-7.65775	-11.96353	H	5.49034	-8.26225	-15.86130
C	-0.27108	-7.58739	-16.92966	H	5.25765	-7.84230	-14.15002
C	-0.94538	-5.77686	-15.30152	H	2.73961	-6.28135	-17.32425
C	0.18278	-6.72480	-15.74365	H	4.12085	-7.35794	-17.63414
C	2.27597	-8.00692	-12.75274	H	2.65186	-7.99878	-16.86178
C	1.36511	-8.92118	-12.20771	H	3.85924	-9.56927	-10.94297
C	0.14145	-9.17009	-12.82313	H	4.64163	-9.46428	-12.53506
C	-0.20707	-8.47736	-13.97954	H	5.32277	-8.58510	-11.14102
C	0.67111	-7.55532	-14.56474	H	2.57453	-7.51620	-9.99468
C	1.94361	-7.36729	-13.97172	H	4.07359	-6.56690	-10.15451
C	3.89821	-4.35389	-15.03338	H	2.56500	-5.99516	-10.91217
C	4.77711	-5.52449	-15.55289	H	4.13033	-6.97987	-12.58304
C	3.91826	-6.80906	-15.54074	H	-1.15005	-8.19792	-16.66723
C	2.81651	-5.09429	-14.25725	H	-0.55743	-6.95029	-17.78235
C	-0.34992	-3.25064	-10.82587	H	0.52053	-8.27333	-17.26646
C	-1.26276	-3.29218	-9.78922	H	-0.63180	-5.16010	-14.44881
C	-3.91586	-3.37454	-6.48220	H	-1.23319	-5.10431	-16.12660
C	-4.55004	-3.13941	-5.42470	H	-1.84497	-6.33988	-15.00401
C	-2.92534	-4.38715	-0.80072	H	1.01747	-6.09662	-16.07585
C	-2.31309	-4.58209	-3.23032	H	1.60454	-9.42437	-11.26833
C	-3.33199	-4.01537	-2.23210	H	-0.56097	-9.87524	-12.38139
C	-8.72157	-5.49210	-4.25890	H	-1.19225	-8.63991	-14.42284
C	-4.81996	-4.41701	-2.49450	H	5.64040	-5.67015	-14.89038
C	-4.96800	-5.72696	-3.28206	H	5.17382	-5.31394	-16.55592
C	-6.42686	-6.15599	-3.40597	H	0.00812	-2.28215	-11.17484
C	-7.25353	-5.08596	-4.12097	H	-3.57186	-3.89526	-0.05523
C	-7.13405	-3.76970	-3.35395	H	-3.00509	-5.47661	-0.64148
C	-5.69219	-3.26200	-3.07980	H	-1.31739	-4.15631	-3.02711
C	-4.98354	0.34022	-2.19802	H	-2.22375	-5.67656	-3.14413
C	-7.20474	-0.23423	-3.13834	H	-2.57072	-4.34189	-4.26912
C	-1.62444	0.78901	-3.37542	H	-3.26345	-2.91826	-2.31620
C	-1.31508	-1.27735	-4.80729	H	-8.82511	-6.46391	-4.76459
C	-2.33358	-0.34989	-4.12180	H	-9.19402	-5.58430	-3.26584
C	-8.01764	0.36292	-6.61664	H	-9.29564	-4.74568	-4.83231
C	-6.86438	-1.61165	-7.69017	H	-5.27676	-4.61085	-1.50593
C	-6.88868	-0.66840	-6.47578	H	-4.53975	-5.61078	-4.29002
C	-3.35033	0.15149	-5.13707	H	-4.38332	-6.51668	-2.78252
C	-2.92808	1.04405	-6.13087	H	-6.85547	-6.32715	-2.40021
C	-3.77310	1.40639	-7.17588	H	-6.50375	-7.11785	-3.93715
C	-5.05047	0.85902	-7.25718	H	-6.82656	-4.94004	-5.13059
C	-5.52609	-0.02025	-6.27615	H	-7.70551	-2.98511	-3.87261
C	-4.67973	-0.33400	-5.18531	H	-7.62365	-3.91067	-2.37276
C	-5.76590	-2.07574	-2.07996	H	-4.89462	1.23030	-2.83885
C	-5.78076	-0.76700	-2.89656	H	-5.50579	0.63694	-1.27536
C	-5.09055	-2.59320	-4.30950	H	-3.97536	0.00696	-1.92266
H	-1.88245	-4.09840	-0.59033	H	-7.85396	-0.98096	-3.61166
H	-6.64289	-2.15522	-1.42249	H	-7.66235	0.05478	-2.17949
H	-1.73315	-6.72174	-9.66564	H	-7.17788	0.65644	-3.78216
H	-0.13337	-6.61662	-11.53369	H	-2.34025	1.47554	-2.89833

H	-0.96501	0.38168	-2.59191	C	-2.91717	-11.20751	-12.07446
H	-0.99329	1.38528	-4.05407	C	-3.68078	-11.54359	-13.35411
H	-0.73106	-0.73518	-5.56848	C	-5.18507	-11.31159	-13.18607
H	-0.61000	-1.68816	-4.06623	C	-5.68276	-12.13074	-11.99359
H	-1.81529	-2.11717	-5.30730	C	-4.96320	-11.83262	-10.64948
H	-2.87350	-0.95848	-3.38531	C	-6.31258	-12.29464	-7.20631
H	-7.89201	0.97242	-7.52623	C	-7.97378	-12.52504	-9.04407
H	-8.99370	-0.14356	-6.69341	C	-5.05499	-9.50738	-5.39403
H	-8.05599	1.05040	-5.75837	C	-4.04571	-8.02283	-7.17234
H	-6.04825	-2.34115	-7.60657	C	-5.03180	-9.16992	-6.89177
H	-7.81662	-2.16149	-7.77146	C	-10.14582	-10.04919	-10.38986
H	-6.72480	-1.04947	-8.62801	C	-8.47914	-8.59060	-11.61482
H	-7.09775	-1.28553	-5.59409	C	-8.67918	-9.60260	-10.47255
H	-1.90788	1.43295	-6.10581	C	-6.40982	-8.82804	-7.44114
H	-3.42437	2.08150	-7.95636	C	-7.08372	-7.71107	-6.92839
H	-5.68219	1.10063	-8.11247	C	-8.27935	-7.26902	-7.48973
H	-4.87705	-2.07582	-1.43500	C	-8.80048	-7.91870	-8.60605
C	-1.75949	-2.09616	-9.15543	C	-8.16000	-9.03521	-9.15883
C	-1.77696	-4.56782	-9.30701	C	-6.98919	-9.52447	-8.52807
H	-1.41817	-1.12844	-9.53080	C	-5.48680	-12.80944	-9.56136
C	-2.64553	-2.14816	-8.12635	C	-6.54560	-12.06975	-8.70540
C	-2.66056	-4.61043	-8.24365	C	-5.40949	-10.48284	-10.11802
H	-3.01276	-1.23060	-7.66869	H	-0.86481	-12.54001	-8.50555
H	-3.03495	-5.57414	-7.89979	H	-5.91162	-13.71484	-10.01725
C	-3.11260	-3.41754	-7.59352	H	-2.52405	-4.47615	-13.48191
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C	-3.13001	-3.89007	-12.79069	H	-1.94868	5.82196	-9.54454
C	-3.05744	-2.53369	-12.80752	H	-3.52452	6.35184	-10.18568
C	-3.84822	-1.72841	-11.89615	H	-2.02019	2.34815	-11.01599
C	-3.80141	-0.36769	-12.03413	H	-0.94653	3.58009	-10.30708
C	-3.77259	0.84115	-12.36066	H	-2.26526	2.89086	-9.35003
C	-2.96297	5.48123	-9.80897	H	-2.44407	4.78364	-11.74839
C	-1.98898	3.22644	-10.36094	H	-8.70256	2.91204	-12.23702
C	-2.90918	4.35294	-10.84818	H	-8.28798	1.48767	-13.22485
C	-8.16078	1.95010	-12.23231	H	-8.64854	1.29460	-11.49245
C	-4.33846	3.90498	-11.25029	H	-4.94198	4.83182	-11.29126
C	-5.00151	2.99847	-10.20264	H	-4.90214	3.45807	-9.20654
C	-6.47924	2.74606	-10.50359	H	-4.46959	2.03564	-10.16163
C	-6.68267	2.15092	-11.89984	H	-7.03730	3.69926	-10.43285
C	-5.99450	3.03658	-12.94196	H	-6.91586	2.07621	-9.74228
C	-1.47301	4.24423	-14.36693	H	-6.19239	1.16471	-11.91941
C	-3.13549	3.64983	-16.11384	H	-6.10887	2.59325	-13.94529
C	1.14551	1.91483	-13.60486	H	-6.51066	4.01505	-12.96970
C	-0.05535	0.44614	-11.93689	H	-0.69184	3.72059	-14.93566
C	-0.21824	1.37636	-13.14988	H	-1.49027	5.29301	-14.70282
C	-4.70647	0.67491	-17.43277	H	-1.19423	4.22839	-13.30526
C	-5.37775	-0.53242	-15.30850	H	-4.14819	3.29668	-16.34596
C	-4.46528	0.54438	-15.92189	H	-3.04921	4.68840	-16.46878
C	-0.97330	0.66954	-14.26392	H	-2.41538	3.03701	-16.67666
C	-0.41301	-0.48734	-14.82185	H	1.82857	1.09542	-13.87900
C	-1.10823	-1.24634	-15.75887	H	1.05617	2.57610	-14.47969
C	-2.39653	-0.87076	-16.13078	H	1.62561	2.48507	-12.79285
C	-3.00519	0.26940	-15.58991	H	0.61737	-0.39469	-12.17148
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C	-4.48427	3.31483	-12.68975	H	-1.02378	0.03031	-11.62428
C	-3.96857	4.29159	-13.78786	H	-0.82861	2.22608	-12.82739
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C	-3.69104	2.04667	-12.96988	H	-5.75307	0.95755	-17.63221
C	-4.67649	-2.41157	-10.95082	H	-4.05305	1.43517	-17.88689
C	-4.75536	-3.79052	-10.92285	H	-5.22502	-0.61363	-14.22408
C	-4.93723	-8.01916	-10.76828	H	-6.43691	-0.28803	-15.49394
C	-5.09487	-9.24271	-10.55297	H	-5.17943	-1.52306	-15.74862
C	-1.46878	-12.72538	-9.40880	H	-4.73745	1.49805	-15.45326
C	-1.99078	-10.26599	-9.46612	H	0.57016	-0.81844	-14.48621
C	-2.58144	-11.68025	-9.56196	H	-0.65960	-2.15364	-16.16833
C	-5.96826	-11.64699	-14.45497	H	-2.95808	-1.49790	-16.82664
C	-3.42367	-11.97320	-10.84369	H	-3.60772	5.23344	-13.35380

H	-4.79784	4.55788	-14.45819	C	2.64306	-2.21954	-15.86566
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H	-1.87945	-13.74616	-9.33938	C	4.60684	-8.04128	-15.31173
H	-0.78411	-12.70097	-10.27421	C	3.22946	-6.97837	-17.08018
H	-1.53657	-10.11850	-8.47291	C	4.25664	-9.04732	-11.89236
H	-1.19549	-10.10345	-10.21004	C	3.14020	-7.03168	-10.84366
H	-2.75021	-9.48672	-9.60606	C	3.45328	-7.76659	-12.15844
H	-3.25089	-11.79266	-8.69296	C	-0.38303	-7.34784	-17.07122
H	-5.61618	-11.04841	-15.31073	C	-0.96748	-5.56205	-15.37968
H	-5.85273	-12.71199	-14.72208	C	0.11388	-6.54417	-15.86126
H	-7.04521	-11.44951	-14.32628	C	2.17418	-8.02632	-12.94153
H	-3.28766	-13.04734	-11.07135	C	1.22897	-8.91970	-12.42051
H	-2.99214	-10.12536	-11.89325	C	-0.01329	-9.08737	-13.02706
H	-1.84828	-11.43578	-12.21196	C	-0.34148	-8.33674	-14.15305
H	-3.51163	-12.60306	-13.62658	C	0.57214	-7.43436	-14.71449
H	-3.29254	-10.93950	-14.19217	C	1.85655	-7.32163	-14.12853
H	-5.34170	-10.24385	-12.95445	C	3.92672	-4.33607	-15.06213
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H	-8.17848	-12.46705	-10.12098	C	-3.96647	-3.39857	-6.47574
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H	-8.71538	-11.90958	-8.51479	C	-2.96154	-4.29305	-0.75836
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H	-7.43049	-8.26994	-11.68228	C	-7.31790	-0.25035	-3.18797
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H	-9.09938	-7.69187	-11.46523	C	-1.39002	-1.25357	-4.77354
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H	-9.70511	-7.53086	-9.07985	C	-6.95995	-0.66825	-6.52053
H	-4.66271	-13.13822	-8.91512	C	-3.42962	0.15789	-5.16759
C	-5.59415	-4.49530	-9.98430	C	-2.99453	1.03020	-6.17387
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C	-4.04161	-5.96991	-11.82316	C	-4.75872	-0.32921	-5.22210
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				H	-1.92414	-3.98441	-0.54869
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				H	-0.09962	-6.59277	-11.53008
				H	7.17299	-2.86808	-12.76413
				H	7.38737	-4.46799	-12.01487
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H	5.14263	-7.93119	-14.36075	C	-2.61683	-2.17947	-8.08583
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H	-1.88295	-6.09623	-15.07750	C	-4.36909	3.93130	-11.29341
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H	1.45705	-9.47134	-11.50562	C	-6.51953	2.77002	-10.58081
H	-0.74152	-9.77652	-12.60178	C	-6.68815	2.15613	-11.97380
H	-1.33671	-8.43921	-14.59196	C	-5.97374	3.02573	-13.01225
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H	5.17949	-5.28131	-16.61466	C	-2.99559	3.59507	-16.10937
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H	-3.61804	-3.80460	-0.01941	C	-0.06452	0.49691	-11.78107
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H	-2.23267	-5.59364	-3.08662	C	-5.26476	-0.56854	-15.33000
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H	-7.31378	0.63526	-3.83931	C	-6.05804	-11.72741	-14.36138
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C	0.01920	-9.13570	-12.85830	H	4.51444	-9.55673	-12.68134
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H	5.23164	-3.68722	-14.03480
H	4.44603	-2.11774	-14.28992
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H	1.84065	-0.80673	-18.09719
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3^{dimer}, triplet

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H	-3.23066	-2.14954	-9.26427	C	-6.57307	-10.30467	-8.50333
H	-2.02465	-6.19455	-8.37833	C	-5.24039	-10.74276	-8.30260
C	-4.24234	-3.09803	-7.63659	C	-3.82397	-13.88380	-9.78771
C	-3.57370	-5.38468	-7.14060	C	-4.71338	-13.25514	-8.68545
H	-4.88703	-2.23895	-7.44530	C	-4.20532	-11.60098	-10.35167
H	-3.67994	-6.29540	-6.55006	H	0.81171	-13.01962	-10.13027
C	-4.41230	-4.27700	-6.86006	H	-4.20170	-14.87123	-10.08824
N	-2.63031	3.56633	-12.28293	H	-2.97111	-3.31008	-12.87879
N	-4.71169	-11.82382	-9.07937	H	-2.85252	-0.84985	-12.79842
C	-3.74266	-2.75721	-12.34078	H	-4.27010	4.87700	-6.67524
C	-3.66090	-1.37428	-12.28578	H	-2.50044	4.70637	-6.65128
C	-4.59806	-0.62386	-11.52479	H	-3.25719	6.03431	-7.56986
C	-4.44732	0.76934	-11.43916	H	-3.45420	1.91205	-8.95786
C	-4.19327	1.98067	-11.42509	H	-2.43149	2.38914	-7.58587
C	-3.35845	4.97279	-7.29012	H	-4.19362	2.34669	-7.40168
C	-3.38227	2.59537	-8.10276	H	-2.52428	4.25122	-9.11944
C	-3.43605	4.06879	-8.52690	H	-8.37261	5.50627	-11.97352
C	-8.07949	4.47175	-12.22404	H	-7.87437	4.43536	-13.30662
C	-4.66111	4.46109	-9.41160	H	-8.94665	3.82170	-12.02372
C	-5.90347	3.60701	-9.11361	H	-4.92751	5.50071	-9.14300
C	-7.13541	4.04338	-9.90397	H	-6.11698	3.64085	-8.03250
C	-6.86096	4.03484	-11.41088	H	-5.68673	2.55683	-9.35667
C	-5.64901	4.92206	-11.70498	H	-7.43678	5.06420	-9.59998
C	-0.83550	5.27917	-12.01104	H	-7.98692	3.38237	-9.66808
C	-2.61234	5.61699	-13.71847	H	-6.60489	3.00138	-11.70236
C	0.98710	2.48645	-10.74587	H	-5.44075	4.92561	-12.78717
C	-0.82758	0.85707	-10.07991	H	-5.90548	5.96345	-11.43292
C	-0.48790	2.09900	-10.92284	H	-0.17519	4.77482	-12.73277

H	-7.71146	0.10032	-2.21142
H	-7.21320	0.69886	-3.81166
H	-4.91097	-2.04025	-1.45923
C	-1.77992	-2.09201	-9.15589
C	-1.80355	-4.56423	-9.29793
H	-1.43557	-1.12833	-9.54059
C	-2.66963	-2.13760	-8.12969
C	-2.69092	-4.60034	-8.23751
H	-3.03683	-1.21564	-7.67525
H	-3.06701	-5.56327	-7.88619
C	-3.14192	-3.40368	-7.59359
N	-2.88839	2.19633	-14.10700
N	-6.34754	-10.64398	-9.06609
C	-3.14259	-3.89879	-12.78745
C	-3.06683	-2.54266	-12.80948
C	-3.85948	-1.73196	-11.90456
C	-3.80954	-0.37193	-12.04809
C	-3.77737	0.83540	-12.37975
C	-4.34479	3.90406	-11.28378
C	-5.99350	3.03097	-12.98009
C	-1.46473	4.22860	-14.39038
C	-3.12070	3.62723	-16.14111
C	-2.25723	1.05224	-14.69741
C	-4.48418	3.30860	-12.72171
C	-3.96243	4.28035	-13.82140
C	-2.83753	3.58152	-14.63370
C	-3.69106	2.03848	-12.99309
C	-4.69296	-2.40940	-10.95968
C	-4.77493	-3.78804	-10.92626
C	-4.96743	-8.01558	-10.75628
C	-5.12761	-9.23810	-10.53716
C	-3.45946	-11.97130	-10.81650
C	-5.71723	-12.13041	-11.96894
C	-4.99913	-11.82841	-10.62487
C	-6.35957	-12.27761	-7.18382
C	-8.01441	-12.51236	-9.02665
H	-6.32441	-8.80291	-8.04681
C	-7.02943	-9.51101	-8.51810
C	-5.52570	-12.80069	-9.53417
C	-6.58698	-12.05733	-8.68448
C	-5.44505	-10.47636	-10.09899
H	-5.93509	-13.72239	-9.97169
H	-2.52927	-4.49309	-13.46944
H	-2.40294	-2.03557	-13.51241
H	-4.95348	4.81774	-11.19949
H	-6.14747	2.62765	-13.99286
H	-6.57537	3.96217	-12.88136
H	-0.66889	3.67545	-14.91493
H	-1.45736	5.26652	-14.75901
H	-1.22132	4.23865	-13.31619
H	-4.07509	3.13181	-16.37963
H	-3.18036	4.67354	-16.47899
H	-2.32370	3.13776	-16.72196
H	-3.58314	5.21186	-13.37528
H	-4.78368	4.56758	-14.49298
H	-5.27878	-1.81749	-10.25331
H	-3.21367	-12.99424	-11.14300
H	-6.80993	-12.06909	-11.85674
H	-5.45968	-13.14322	-12.32027
H	-7.11127	-11.74725	-6.57795
H	-6.43382	-13.34977	-6.94236
H	-5.36177	-11.92197	-6.88320
H	-8.22416	-12.39786	-10.10081

H	-8.15025	-13.57188	-8.75909
H	-8.76315	-11.92646	-8.46983
H	-4.69175	-13.09953	-8.88041
C	-5.61895	-4.48715	-9.98813
C	-3.99465	-4.59372	-11.85664
H	-6.19997	-3.89423	-9.27666
C	-5.68103	-5.84437	-9.95669
C	-4.06297	-5.97259	-11.81533
H	-6.31608	-6.35558	-9.22999
H	-3.45411	-6.56158	-12.50435
C	-4.88940	-6.65433	-10.86816
H	2.64239	-2.81746	-15.89445
H	4.09569	-2.58485	-13.74560
H	0.88781	-7.08825	-14.14846
H	2.08701	-8.39675	-14.34927
H	-6.38327	2.29432	-12.26056
H	-4.69255	3.17662	-10.53435
H	-3.29657	4.15461	-11.05699
H	-1.60525	0.53521	-13.97165
H	-3.00243	0.31553	-15.04763
H	-1.63965	1.36115	-15.55175
H	-3.62083	-0.40014	-5.36113
H	-5.19816	-0.52669	-6.16919
H	-7.17098	-4.54142	-4.11142
H	-4.80774	-5.21979	-3.20689
H	-3.84731	-4.02915	-2.29223
H	-7.57680	-8.95364	-9.29943
H	-2.92830	-11.76199	-9.87540
H	-3.09832	-11.26311	-11.57819
H	-5.41797	-11.40505	-12.74127
H	5.17028	-3.92140	-13.26117
H	2.03590	-7.44203	-12.84030
H	-7.74899	-9.83921	-7.75497

Truncated 2^{dimer}, triplet

N	2.87589	-6.46206	-14.55781
N	-5.12343	-1.19303	-4.17423
C	-1.32898	-5.75718	-9.99909
C	-0.44857	-5.70731	-11.03512
C	0.10498	-4.44342	-11.49540
C	1.02712	-4.46558	-12.50918
C	1.90014	-4.63583	-13.39380
H	2.63171	-2.81465	-15.93055
C	3.31611	-3.61040	-16.26365
C	4.73347	-8.04615	-15.10246
C	3.31537	-7.14341	-16.92832
H	2.05534	-7.43530	-12.88170
H	0.89994	-7.07714	-14.18217
C	1.94297	-7.37991	-13.97954
C	3.90270	-4.37109	-15.04472
C	4.77972	-5.54365	-15.56298
C	3.91910	-6.82703	-15.54871
C	2.81978	-5.10886	-14.26775
C	-0.34466	-3.25295	-10.84155
C	-1.25699	-3.29036	-9.80431
C	-3.90777	-3.35963	-6.49531
C	-4.54081	-3.12049	-5.43805
C	-7.12458	-3.74129	-3.36481
C	-5.68158	-3.23592	-3.09241
C	-4.96462	0.36635	-2.21858
C	-7.18830	-0.20500	-3.15497
H	-3.57737	-0.40632	-5.36756
H	-5.15748	-0.53434	-6.16990

C	-4.66627	-0.31412	-5.20497
C	-5.75214	-2.04760	-2.09482
C	-5.76520	-0.74041	-2.91397
C	-5.07965	-2.57075	-4.32379
H	-6.61991	-2.12143	-1.42346
H	-1.73694	-6.71710	-9.67181
H	-0.13462	-6.62352	-11.53970
H	2.75001	-4.27459	-16.93213
H	4.13063	-3.14881	-16.84510
H	4.12822	-8.96598	-15.11040
H	5.57941	-8.20230	-15.78997
H	5.13430	-7.90284	-14.08687
H	2.72497	-6.30159	-17.31631
H	4.11330	-7.37077	-17.65267
H	2.65153	-8.02112	-16.87124
H	5.63210	-5.68453	-14.87856
H	5.19515	-5.33993	-16.56025
H	0.02972	-2.28766	-11.19040
H	-7.78192	-2.94204	-3.73299
H	-7.56101	-4.14628	-2.43745
H	-4.99794	1.31168	-2.78183
H	-5.38917	0.56062	-1.22130
H	-3.91058	0.07250	-2.09494
H	-7.83020	-0.95153	-3.64154
H	-7.65573	0.08441	-2.20057
H	-7.16314	0.68738	-3.80093
H	-4.84923	-2.05556	-1.46230
C	-1.75100	-2.09185	-9.17312
C	-1.77313	-4.56389	-9.31862
H	-1.40980	-1.12731	-9.55845
C	-2.63634	-2.13968	-8.14324
C	-2.65600	-4.60228	-8.25452
H	-3.00296	-1.21867	-7.68642
H	-3.03014	-5.56601	-7.90334
C	-3.10529	-3.40693	-7.60699
N	-2.88395	2.20266	-14.11332
N	-6.31096	-10.64782	-9.07640
C	-3.12743	-3.89456	-12.80150
C	-3.05291	-2.53834	-12.82190
C	-3.84243	-1.72962	-11.91248
C	-3.79425	-0.36934	-12.05425
C	-3.76449	0.83849	-12.38430
C	-4.32988	3.90509	-11.28153
C	-5.98499	3.03303	-12.97213
C	-1.46321	4.23654	-14.39976
C	-3.12604	3.63628	-16.14437
H	-1.59730	0.54326	-13.98639
H	-3.00084	0.32240	-15.05458
C	-2.25432	1.05996	-14.70804
C	-4.47483	3.31158	-12.71972
C	-3.95854	4.28535	-13.82020
C	-2.83648	3.58865	-14.63823
C	-3.68178	2.04253	-12.99627
C	-4.67134	-2.40913	-10.96507
C	-4.75201	-3.78789	-10.93329
C	-4.94022	-8.01583	-10.76860
C	-5.09844	-9.23880	-10.55057
H	-2.89425	-11.76219	-9.90168
C	-3.42917	-11.97017	-10.84088
H	-3.07180	-11.26030	-11.60284
H	-5.39672	-11.40251	-12.75646
C	-5.69165	-12.12955	-11.98402
C	-4.96814	-11.82887	-10.64256

C	-6.31368	-12.28418	-7.19646
C	-7.97608	-12.51768	-9.03263
H	-6.28448	-8.80561	-8.05945
H	-7.54729	-8.96135	-9.30077
C	-6.99150	-9.51623	-8.52391
C	-5.48928	-12.80316	-9.55105
C	-6.54761	-12.06192	-8.69582
C	-5.41298	-10.47795	-10.11285
H	-5.89967	-13.72460	-9.98820
H	-2.51700	-4.48736	-13.48738
H	-2.39288	-2.02967	-13.52730
H	-4.93915	4.81803	-11.19353
H	-6.14291	2.63145	-13.98499
H	-6.56731	3.96348	-12.86918
H	-0.66915	3.68509	-14.92877
H	-1.45838	5.27516	-14.76647
H	-1.21517	4.24480	-13.32662
H	-4.08084	3.14010	-16.37962
H	-3.18833	4.68304	-16.48040
H	-2.33091	3.14866	-16.72931
H	-3.57809	5.21648	-13.37426
H	-4.78284	4.57297	-14.48785
H	-5.25483	-1.81875	-10.25549
H	-3.18401	-12.99232	-11.17031
H	-6.78393	-12.06988	-11.86701
H	-5.43422	-13.14142	-12.33814
H	-7.06295	-11.75502	-6.58650
H	-6.38656	-13.35666	-6.95607
H	-5.31476	-11.92849	-6.89960
H	-8.19030	-12.40201	-10.10580
H	-8.11015	-13.57761	-8.76581
H	-8.72310	-11.93300	-8.47223
H	-4.65232	-13.10222	-8.90126
C	-5.59148	-4.48906	-9.99262
C	-3.97497	-4.59156	-11.86812
H	-6.17026	-3.89766	-9.27808
C	-5.65228	-5.84637	-9.96288
C	-4.04195	-5.97055	-11.82851
H	-6.28396	-6.35926	-9.23444
H	-3.43547	-6.55802	-12.52091
C	-4.86381	-6.65435	-10.87885
C	4.63756	-3.32105	-14.19091
H	3.92331	-2.56462	-13.83243
H	5.11381	-3.77844	-13.30916
H	5.41516	-2.81436	-14.78460
H	-7.70336	-9.84590	-7.75432
H	-6.37097	2.29465	-12.25235
H	-4.67366	3.17634	-10.53156
H	-3.28093	4.15648	-11.05913
H	-1.64227	1.37063	-15.56568
H	-7.11875	-4.53957	-4.12339
H	-4.88672	0.72768	-4.93654
C	-4.87370	-4.45758	-2.61652
H	-5.33615	-4.90147	-1.72034
H	-4.84598	-5.21962	-3.40988
H	-3.83393	-4.18518	-2.37519
H	2.09748	-8.38543	-14.39355

Truncated 2^{dimer}, quintet

N	2.77736	-6.49537	-14.64388
N	-5.26216	-1.22226	-4.18020
C	-1.29729	-5.77152	-9.93915

C	-0.41989	-5.71423	-10.99233	C	-3.04978	-2.46626	-12.79020
C	0.09174	-4.45316	-11.46148	C	-3.82906	-1.69953	-11.86040
C	1.01375	-4.47140	-12.53113	C	-3.77090	-0.29426	-11.97432
C	1.86856	-4.66672	-13.40700	C	-3.74833	0.88613	-12.34638
C	4.74526	-3.47052	-14.21996	C	-4.33207	3.98336	-11.27005
C	3.29955	-3.62081	-16.29988	C	-5.93764	3.11965	-13.00872
C	4.57867	-8.12392	-15.24494	C	-1.34910	4.28320	-14.25281
C	3.17824	-7.12866	-17.03493	C	-2.92482	3.69904	-16.08170
H	1.98339	-7.49144	-12.96513	C	-2.16987	1.10524	-14.62949
H	0.79600	-7.05860	-14.21441	C	-4.43299	3.38275	-12.71001
C	1.83516	-7.39735	-14.05679	C	-3.87097	4.34458	-13.79999
C	3.86911	-4.42043	-15.09694	C	-2.71208	3.64309	-14.56318
C	4.70453	-5.61229	-15.64120	C	-3.63223	2.11480	-12.94881
C	3.80098	-6.86761	-15.65184	C	-4.62435	-2.37660	-10.93236
C	2.77612	-5.14091	-14.32425	C	-4.68152	-3.78875	-10.91434
C	-0.34436	-3.28415	-10.83293	C	-4.80082	-8.04223	-10.78706
C	-1.25747	-3.32520	-9.75314	C	-4.99571	-9.24432	-10.56538
C	-3.93634	-3.41494	-6.43531	C	-3.45818	-12.08544	-10.87981
C	-4.55320	-3.15682	-5.39072	C	-5.72571	-12.11927	-12.01766
C	-4.80912	-4.36151	-2.41021	C	-4.98760	-11.86027	-10.67516
C	-7.14385	-3.85660	-3.28817	C	-6.33344	-12.27530	-7.22208
C	-5.72889	-3.26580	-3.03746	C	-8.02081	-12.39880	-9.04643
C	-5.21081	0.40080	-2.27122	C	-6.86972	-9.46088	-8.50712
C	-7.38981	-0.32272	-3.20663	C	-5.55856	-12.81334	-9.58870
C	-4.80609	-0.35497	-5.22101	C	-6.56753	-12.02329	-8.71669
C	-5.86489	-2.04948	-2.07951	C	-5.35456	-10.49543	-10.12940
C	-5.94065	-0.76947	-2.93983	H	-6.02383	-13.70553	-10.03152
C	-5.15321	-2.60764	-4.28175	H	-2.47873	-4.40529	-13.48606
H	-6.73059	-2.14380	-1.40775	H	-2.41668	-1.93701	-13.50428
H	-1.68433	-6.73642	-9.60208	H	-4.94040	4.89887	-11.20138
H	-0.09350	-6.62918	-11.49029	H	-6.06743	2.71636	-14.02502
H	2.69508	-4.25884	-16.95915	H	-6.51666	4.05443	-12.92591
H	4.12059	-3.18603	-16.89342	H	-0.53251	3.72935	-14.74381
H	3.94389	-9.02346	-15.27012	H	-1.32039	5.32363	-14.61336
H	5.41315	-8.28954	-15.94405	H	-1.15589	4.28472	-13.16845
H	4.99331	-8.02025	-14.22997	H	-3.86715	3.20578	-16.36798
H	2.61269	-6.25886	-17.39702	H	-2.96930	4.74779	-16.41429
H	3.96378	-7.36226	-17.77074	H	-2.10161	3.21419	-16.62889
H	2.48669	-7.98595	-16.99578	H	-3.51400	5.28378	-13.35137
H	5.55117	-5.79740	-14.96120	H	-4.66711	4.61896	-14.50649
H	5.12568	-5.40442	-16.63552	H	-5.21326	-1.81074	-10.20808
H	0.01370	-2.31497	-11.18643	H	-3.26862	-13.11647	-11.21859
H	-5.24253	-4.72205	-1.46362	H	-6.81378	-12.00765	-11.89816
H	-7.82885	-3.10380	-3.69976	H	-5.51810	-13.13941	-12.38135
H	-7.57069	-4.23786	-2.34603	H	-7.04983	-11.71687	-6.59881
H	-5.28713	1.32508	-2.86459	H	-6.45839	-13.34558	-6.99365
H	-5.65886	0.60309	-1.28591	H	-5.31517	-11.97453	-6.93017
H	-4.14417	0.16908	-2.12470	H	-8.23547	-12.26280	-10.11718
H	-7.98240	-1.11710	-3.67986	H	-8.20996	-13.45225	-8.78727
H	-7.88266	-0.03790	-2.26375	H	-8.73151	-11.77946	-8.47598
H	-7.40978	0.55329	-3.87510	H	-4.73571	-13.16641	-8.94796
H	-4.96535	-1.98953	-1.44626	C	-5.49185	-4.50148	-9.98130
C	-1.73339	-2.13991	-9.12040	C	-3.90338	-4.54536	-11.85307
C	-1.74372	-4.58869	-9.27698	H	-6.07589	-3.93233	-9.25334
H	-1.39700	-1.17163	-9.50015	C	-5.52269	-5.87037	-9.96518
C	-2.61235	-2.19635	-8.07013	C	-3.94394	-5.95923	-11.82300
C	-2.64642	-4.62959	-8.18725	H	-6.13669	-6.40222	-9.23625
H	-2.96844	-1.27854	-7.59964	H	-3.32936	-6.52286	-12.52732
H	-3.01042	-5.59737	-7.83779	C	-4.73246	-6.63869	-10.89192
C	-3.07956	-3.45756	-7.56022	H	-5.39797	-11.40208	-12.78657
N	-2.79195	2.25642	-14.04592	H	2.65367	-2.79979	-15.94948
N	-6.25917	-10.61950	-9.08359	H	5.55701	-3.03730	-14.82583
C	-3.09135	-3.83610	-12.78256	H	-6.35365	2.38697	-12.29938

H	-7.09611	-4.68995	-4.00759
H	-4.70480	-5.21727	-3.09555
H	-5.07567	0.68426	-4.98887
H	-3.06452	-11.39035	-11.63776
H	-2.91001	-11.91428	-9.94063
H	-7.56613	-9.76169	-7.71180
H	1.94076	-8.39515	-14.50425
H	-1.51646	1.40985	-15.45865
H	-2.91780	0.38971	-15.01777
H	-1.55168	0.56397	-13.89248
H	4.13464	-2.64892	-13.81421
H	5.18636	-4.01881	-13.37379
H	-4.70186	3.25818	-10.52869
H	-3.28951	4.23099	-11.01541
H	-3.80471	-3.95806	-2.21173
H	-5.25694	-0.61584	-6.19498
H	-3.70881	-0.40591	-5.34637
H	-7.43302	-8.87811	-9.25852
H	-6.11716	-8.78387	-8.06519

H	1.39724	-2.94650	-18.91560
H	3.32630	-8.48283	-16.96500
H	4.15289	-7.67306	-18.31332
H	4.36752	-7.06855	-16.64634
H	0.58309	-6.59546	-18.69996
H	1.94381	-7.45399	-19.47288
H	1.08938	-8.19426	-18.09884
H	3.98753	-5.09409	-17.99062
H	2.65457	-5.05963	-19.14712
H	-0.28073	-2.01703	-12.41523
H	-1.55543	-2.05173	-10.35740
H	-7.78626	-6.07964	-1.60685
H	-9.86314	-4.74618	-4.46941
H	-9.81086	-5.91715	-3.12294
H	-8.39753	-0.02739	-2.84900
H	-9.07811	-0.86574	-1.43957
H	-7.35205	-1.07274	-1.84738
H	-10.44543	-2.75514	-4.37773
H	-10.85989	-1.74353	-2.96839
H	-10.08666	-1.01374	-4.39561
H	-8.05935	-3.33044	-1.42620
C	-2.42743	-4.24740	-8.96557
C	-3.10660	-3.06640	-8.51210
C	-2.78263	-5.46274	-8.28828
H	-2.89524	-2.10818	-8.98376
H	-2.30110	-6.39666	-8.57743
C	-4.07371	-3.09740	-7.54545
C	-3.73791	-5.51063	-7.30799
H	-4.59327	-2.17899	-7.26492
H	-3.98813	-6.46290	-6.83484
C	-4.45169	-4.33130	-6.90310
N	-2.65694	3.61968	-12.37986
N	-5.00837	-11.74499	-9.26605
C	-3.91799	-2.54733	-12.43576
C	-3.86502	-1.18212	-12.37888
C	-4.62849	-0.44412	-11.40369
C	-4.45775	0.91214	-11.31518
C	-4.17303	2.12981	-11.32125
H	-3.33192	4.27487	-8.79521
C	-4.27185	4.59728	-9.26864
C	-5.45187	5.14526	-11.45274
C	-0.71356	5.18620	-12.30643
C	-2.65522	5.70253	-13.76974
H	-1.72785	1.74564	-12.59474
H	-2.94821	2.12082	-13.83102
C	-2.15177	2.56255	-13.20511
C	-4.11324	4.67268	-10.81902
C	-2.97711	5.64750	-11.23040
C	-2.23359	5.04141	-12.44741
C	-3.67013	3.37609	-11.47257
C	-5.49603	-1.20614	-10.54973
C	-5.52413	-2.57334	-10.61330
C	-4.71232	-3.32494	-11.52798
C	-4.13146	-8.95207	-11.04859
C	-4.10362	-10.17895	-10.80582
H	-1.60544	-12.50029	-10.42080
C	-2.19300	-12.71994	-11.32526
H	-4.35239	-12.27054	-13.05654
C	-4.51654	-13.05220	-12.29873
C	-3.71831	-12.73562	-11.00358
C	-4.78048	-13.48598	-7.49261
C	-6.51955	-13.74361	-9.25132
H	-4.94350	-9.93764	-8.19983

Truncated 3^{dimer}, singlet

N	1.81581	-6.20869	-16.25556
N	-7.69945	-2.45218	-4.16782
C	-0.97826	-5.41563	-10.65237
C	-0.26658	-5.40713	-11.82123
C	-0.01306	-4.18054	-12.53650
C	0.60579	-4.22634	-13.75982
C	1.14835	-4.40049	-14.87385
H	4.10002	-3.36949	-16.30183
C	3.24925	-2.95145	-16.86103
C	1.03139	-3.45624	-18.00935
C	3.64225	-7.50150	-17.35265
C	1.45517	-7.23974	-18.50980
H	1.78707	-7.09158	-14.34404
H	0.20560	-6.98494	-15.14671
C	1.28189	-7.15788	-15.32431
C	2.22039	-4.06988	-17.21871
C	2.89349	-5.17584	-18.08054
C	2.44701	-6.56131	-17.55224
C	1.70308	-4.85318	-16.02378
C	-0.47849	-2.97004	-11.91952
C	-1.19836	-3.00027	-10.75515
C	-1.53071	-4.22149	-10.07744
C	-5.45531	-4.32003	-5.96828
C	-6.36318	-4.17221	-5.11957
H	-6.37164	-5.00801	-1.84902
C	-7.17311	-5.56150	-2.36110
C	-9.20265	-5.39958	-3.88282
C	-8.06450	-4.59356	-3.19960
C	-8.36270	-0.96412	-2.27096
C	-10.11035	-1.91178	-3.75759
H	-6.10945	-1.33494	-4.97973
H	-7.36856	-1.80496	-6.14134
C	-7.19806	-1.48533	-5.09764
C	-8.69505	-3.48753	-2.31181
C	-8.72994	-2.17696	-3.13323
C	-7.29740	-3.77224	-4.22478
H	-9.69418	-3.76776	-1.94835
H	-1.17072	-6.37817	-10.17893
H	0.09838	-6.34485	-12.24562
H	3.62568	-2.48201	-17.78366
H	0.31748	-4.23668	-18.31336

H	-6.39722	-10.16008	-9.19664	C	1.72641	-2.93453	-17.80121
C	-5.66878	-10.68975	-8.55623	C	3.10027	-7.56598	-17.61735
C	-4.05338	-13.79418	-9.91759	C	1.22837	-6.49380	-18.85827
C	-5.11335	-13.19411	-8.96070	H	1.02502	-7.04531	-14.70441
C	-4.24085	-11.45500	-10.37666	H	-0.33658	-6.46404	-15.68814
H	-4.39923	-14.73983	-10.35886	C	0.69059	-6.86946	-15.74210
H	-3.29397	-3.05181	-13.17179	C	2.62591	-3.91420	-16.99804
H	-3.21769	-0.62994	-13.06360	C	3.12113	-5.04058	-17.94668
H	-4.55026	5.58557	-8.86993	C	2.24428	-6.29765	-17.72243
H	-5.36735	5.22872	-12.54584	C	1.79803	-4.68759	-15.98966
H	-5.73918	6.13030	-11.04940	C	-0.22168	-2.91071	-11.72092
H	-0.18165	4.76325	-13.17309	C	-0.97894	-2.95999	-10.55913
H	-0.44243	6.25156	-12.23944	C	-1.60255	-4.14962	-10.13121
H	-0.35309	4.67845	-11.39836	C	-5.41212	-4.31113	-5.86605
H	-3.74347	5.64637	-13.91897	C	-6.30252	-4.15608	-5.01907
H	-2.35980	6.76334	-13.77716	H	-6.29540	-4.63300	-1.64068
H	-2.17010	5.21177	-14.62886	C	-7.03172	-5.30971	-2.10065
H	-2.26611	5.74790	-10.39543	C	-9.02804	-5.50611	-3.65677
H	-3.35817	6.65485	-11.45130	C	-7.98794	-4.52327	-3.05133
H	-6.11302	-0.67688	-9.81987	C	-8.59730	-0.85671	-2.52077
H	-6.17248	-3.10237	-9.91618	C	-10.25375	-2.08510	-3.90598
H	-1.88190	-13.69961	-11.72135	H	-6.32553	-1.33557	-5.23044
H	-5.59669	-13.10168	-12.09778	H	-7.56207	-2.03219	-6.30004
H	-4.19504	-14.01994	-12.71755	C	-7.39948	-1.58557	-5.30247
H	-5.54036	-13.07006	-6.81258	C	-8.74026	-3.39054	-2.30132
H	-4.74596	-14.57377	-7.32414	C	-8.86341	-2.17596	-3.25522
H	-3.80212	-13.06096	-7.21907	C	-7.28182	-3.75208	-4.15019
H	-6.80599	-13.57718	-10.30038	H	-9.72310	-3.71952	-1.93424
H	-6.55507	-14.82571	-9.05050	H	-1.91657	-6.23275	-10.63464
H	-7.27436	-13.25588	-8.61358	H	-0.57225	-6.17317	-12.69469
H	-3.14336	-14.02217	-9.34108	H	4.40730	-2.64119	-17.18639
C	-4.63227	-4.74824	-11.47594	H	0.89355	-3.46690	-18.28400
C	-5.32088	-5.51511	-10.47667	H	2.31384	-2.42550	-18.58325
C	-3.79406	-5.49838	-12.36740	H	2.48083	-8.46294	-17.45876
H	-5.96252	-5.00944	-9.75617	H	3.66810	-7.71628	-18.54906
H	-3.23665	-4.97821	-13.14547	H	3.81505	-7.48817	-16.78347
C	-5.15435	-6.86529	-10.34484	H	0.60155	-5.59947	-18.99258
C	-3.62311	-6.85150	-12.25695	H	1.75019	-6.69555	-19.80673
H	-5.66790	-7.40383	-9.54585	H	0.56182	-7.34705	-18.65425
H	-2.95411	-7.37577	-12.94276	H	4.16547	-5.28782	-17.70062
C	-4.28372	-7.60196	-11.22627	H	3.10725	-4.72390	-18.99926
H	-1.36339	2.94694	-13.86652	H	0.24741	-1.97525	-12.03271
H	2.77810	-2.17502	-16.23848	H	-1.09713	-2.05150	-9.96520
H	0.48741	-2.72490	-17.39152	H	-7.61059	-5.80108	-1.30261
H	-6.25840	4.42855	-11.23381	H	-9.73673	-4.98254	-4.31412
H	-5.05760	3.87515	-8.99789	H	-9.59909	-6.00440	-2.85591
H	-8.78646	-6.15384	-4.56900	H	-8.69009	0.01018	-3.19389
H	-6.70589	-6.31592	-3.01274	H	-9.32853	-0.72450	-1.70796
H	-7.69912	-0.52010	-4.94409	H	-7.58692	-0.84773	-2.08294
H	-6.20283	-11.09739	-7.68707	H	-10.51286	-3.01267	-4.43649
H	-1.96567	-11.94922	-12.07799	H	-11.02285	-1.89863	-3.14010
H	1.41228	-8.17756	-15.71110	H	-10.29558	-1.25807	-4.63286

Truncated 3^{dimer}, triplet

N	1.57734	-5.98312	-16.43391
N	-7.80637	-2.47196	-4.25502
C	-1.41481	-5.30592	-10.91563
C	-0.67181	-5.27353	-12.08489
C	-0.06037	-4.06723	-12.52426
C	0.65136	-4.08354	-13.73631
C	1.22910	-4.26582	-14.81649
H	4.48715	-3.79664	-15.81968
C	3.82457	-3.12392	-16.38558

C	1.72641	-2.93453	-17.80121
C	3.10027	-7.56598	-17.61735
C	1.22837	-6.49380	-18.85827
H	1.02502	-7.04531	-14.70441
H	-0.33658	-6.46404	-15.68814
C	0.69059	-6.86946	-15.74210
C	2.62591	-3.91420	-16.99804
C	3.12113	-5.04058	-17.94668
C	2.24428	-6.29765	-17.72243
C	1.79803	-4.68759	-15.98966
C	-0.22168	-2.91071	-11.72092
C	-0.97894	-2.95999	-10.55913
C	-1.60255	-4.14962	-10.13121
C	-5.41212	-4.31113	-5.86605
C	-6.30252	-4.15608	-5.01907
H	-6.29540	-4.63300	-1.64068
C	-7.03172	-5.30971	-2.10065
C	-9.02804	-5.50611	-3.65677
C	-7.98794	-4.52327	-3.05133
C	-8.59730	-0.85671	-2.52077
C	-10.25375	-2.08510	-3.90598
H	-6.32553	-1.33557	-5.23044
H	-7.56207	-2.03219	-6.30004
C	-7.39948	-1.58557	-5.30247
C	-8.74026	-3.39054	-2.30132
C	-8.86341	-2.17596	-3.25522
C	-7.28182	-3.75208	-4.15019
H	-9.72310	-3.71952	-1.93424
H	-1.91657	-6.23275	-10.63464
H	-0.57225	-6.17317	-12.69469
H	4.40730	-2.64119	-17.18639
H	0.89355	-3.46690	-18.28400
H	2.31384	-2.42550	-18.58325
H	2.48083	-8.46294	-17.45876
H	3.66810	-7.71628	-18.54906
H	3.81505	-7.48817	-16.78347
H	0.60155	-5.59947	-18.99258
H	1.75019	-6.69555	-19.80673
H	0.56182	-7.34705	-18.65425
H	4.16547	-5.28782	-17.70062
H	3.10725	-4.72390	-18.99926
H	0.24741	-1.97525	-12.03271
H	-1.09713	-2.05150	-9.96520
H	-7.61059	-5.80108	-1.30261
H	-9.73673	-4.98254	-4.31412
H	-9.59909	-6.00440	-2.85591
H	-8.69009	0.01018	-3.19389
H	-9.32853	-0.72450	-1.70796
H	-7.58692	-0.84773	-2.08294
H	-10.51286	-3.01267	-4.43649
H	-11.02285	-1.89863	-3.14010
H	-10.29558	-1.25807	-4.63286
H	-8.15050	-3.08841	-1.42138
C	-2.49918	-4.17556	-8.96058
C	-3.29764	-3.05880	-8.63978
C	-2.65934	-5.33993	-8.18219
H	-3.22396	-2.15327	-9.24318
H	-2.04190	-6.21469	-8.39599
C	-4.23974	-3.11114	-7.62444
C	-3.58910	-5.40741	-7.15512
H	-4.87498	-2.24661	-7.42431
H	-3.69853	-6.32332	-6.57042
C	-4.41953	-4.29731	-6.86089

N	-2.60021	3.57153	-12.32910
N	-4.73812	-11.80826	-9.04513
C	-3.77292	-2.73739	-12.38064
C	-3.68422	-1.35937	-12.33713
C	-4.58682	-0.59545	-11.53895
C	-4.42609	0.78766	-11.46451
C	-4.16778	2.00145	-11.45834
H	-3.71437	4.21220	-8.88604
C	-4.61814	4.48090	-9.45408
C	-5.60146	4.94703	-11.74986
C	-0.79241	5.27411	-12.07476
C	-2.58128	5.61981	-13.76802
H	-1.54675	1.75269	-12.35711
H	-2.58292	2.03507	-13.77348
C	-1.91903	2.53338	-13.04372
C	-4.30840	4.55585	-10.98265
C	-3.19494	5.59629	-11.28577
C	-2.27116	5.01809	-12.38752
C	-3.71545	3.28459	-11.55982
C	-5.59894	-1.29743	-10.82718
C	-5.66238	-2.67709	-10.87103
C	-4.74450	-3.44382	-11.63015
C	-4.28537	-9.10232	-11.11587
C	-4.21188	-10.30449	-10.81672
H	-1.59708	-12.51778	-10.82492
C	-2.34183	-12.81333	-11.57959
C	-4.79035	-13.30367	-12.04279
C	-3.77187	-12.86640	-10.95399
C	-4.15900	-13.46054	-7.26394
C	-6.16013	-13.83553	-8.68989
H	-4.52622	-9.94866	-8.09057
H	-6.14004	-10.25626	-8.76880
C	-5.28048	-10.73571	-8.26551
C	-3.83590	-13.85907	-9.76068
C	-4.74138	-13.24343	-8.66452
C	-4.21579	-11.56913	-10.30517
H	-4.19264	-14.85267	-10.06770
H	-3.02387	-3.29272	-12.94661
H	-2.89219	-0.84406	-12.88378
H	-4.98728	5.45457	-9.09454
H	-5.41061	5.04257	-12.82867
H	-5.99125	5.90924	-11.37862
H	-0.13423	4.87618	-12.86306
H	-0.60516	6.35709	-12.00378
H	-0.50658	4.80890	-11.11844
H	-3.63789	5.47798	-14.03895
H	-2.36523	6.69960	-13.77182
H	-1.96547	5.14900	-14.55129
H	-2.59815	5.76311	-10.37541
H	-3.61070	6.57052	-11.58041
H	-6.31675	-0.73067	-10.23023
H	-6.44027	-3.18815	-10.30087
H	-2.06817	-13.80223	-11.98052
H	-5.80854	-13.37073	-11.63354
H	-4.51401	-14.28880	-12.45349
H	-4.80881	-13.03654	-6.48233
H	-4.06039	-14.53856	-7.06196
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H	-6.62350	-13.72881	-9.68137
H	-6.13285	-14.90645	-8.43433
H	-6.81028	-13.33007	-7.95764
H	-2.82379	-13.99240	-9.34727
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C	-5.17156	-5.58409	-10.40516
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H	-5.33426	-7.44262	-9.34349
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H	-4.81087	-12.57527	-12.86858
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H	-6.48290	-6.08224	-2.66132
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H	-6.38027	4.18021	-11.61466
H	-5.38794	3.71922	-9.25501
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Truncated 3^{dimer}, quintet

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C	-8.91093	-2.13959	-3.29196
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H	0.31066	-1.97668	-11.98105	H	-5.05363	5.45506	-9.09348
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H	-3.67952	-6.26671	-6.52257	H	-6.61419	-13.72428	-9.62520
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N	-2.63424	3.57254	-12.30513	H	-6.77054	-13.30707	-7.90284
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C	-4.60428	-0.61364	-11.53615	C	-4.24688	-5.70431	-12.65068
C	-4.45418	0.78002	-11.45637	H	-5.44440	-5.01785	-9.53622
C	-4.20160	1.99179	-11.44636	H	-3.96524	-5.21222	-13.58397
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C	-5.65515	4.93236	-11.74698	C	-4.10870	-7.08028	-12.54426
C	-0.84095	5.28799	-12.03733	H	-5.22061	-7.45851	-9.32829
C	-2.61236	5.61394	-13.75310	H	-3.72463	-7.66280	-13.38426
H	-1.58010	1.75475	-12.32877	C	-4.44531	-7.74553	-11.33922
H	-2.59833	2.04281	-13.75742	H	3.47531	-2.33864	-15.65986
C	-1.94453	2.53799	-13.01618	H	1.31734	-2.13571	-17.10505
C	-4.36144	4.55165	-10.97545	H	0.62054	-7.80296	-16.27112
C	-3.25480	5.59962	-11.27908	H	-1.07980	2.96000	-13.54648
C	-2.31422	5.02070	-12.36638	H	-5.44119	3.71629	-9.24702
C	-3.75647	3.28290	-11.54377	H	-6.42856	4.15960	-11.61393
C	-5.64157	-1.31504	-10.87143	H	-8.03155	-0.62980	-5.30391
C	-5.70176	-2.69937	-10.92474	H	-8.48737	-6.25160	-4.24470
C	-4.74944	-3.45288	-11.64139	H	-6.31739	-4.52801	-1.62443
C	-4.28156	-9.12689	-11.14893	H	-5.55910	-11.08933	-7.28183
C	-4.20825	-10.32378	-10.84218	H	-2.34332	-12.13174	-12.43914
C	-2.36404	-12.85513	-11.60919	H	-4.85571	-12.62899	-12.85626
C	-4.82138	-13.34568	-12.02061	H	-3.77241	4.22290	-8.87485
C	-3.78289	-12.89465	-10.95668	H	4.49179	-3.79800	-15.78774
C	-4.10979	-13.44155	-7.25124	H	-6.46714	-5.99416	-2.62708
C	-6.13487	-13.82299	-8.64053				
H	-4.47339	-9.93902	-8.10859				

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