Supporting Information for

Phenothiazine Radical Cation Excited States as Super-oxidants for

Energy Demanding Reactions

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1. Materials, Synthesis, and Characterization

1.1 Materials

All chemicals were obtained from commercial suppliers and used as received unless otherwise noted. Column chromatography was performed using silica gel from Sorbent Technologies. 1H and 13C NMR spectra were recorded at ambient temperature at 500 MHz or 126 MHz, respectively, using a Bruker Avance III spectrometer with chemical shifts reported in ppm relative to TMS. NMR resonance multiplicities are reported with the following abbreviations: s = singlet, d = doublet, and m = multiplet, and coupling constants are reported in Hz. High resolution electrospray ionization (ESI) mass spectra were obtained on an Agilent 6210A LC-TOF.

1.2 Synthesis and Characterization

The synthesis and characterization of PTZ-Per, PTZ-BE, and PTZ-ACN are described in detail below. Molecules 3 and 4 and DPA were purchased from Sigma-Aldrich and used as received. PTZ,¹ 1,² 2,³ Per,⁴ PTZ-DPA,⁵ 5,⁶ and ACN⁷ were prepared as described previously. The synthesis of PTZ-Per, PTZ-BE, and PTZ-ACN is described below.



Scheme 1. Structures of molecules examined in this study.



PTZ-Per. 10-(4-bromophenyl)-10*H*-phenothiazine² (0.091 g, 0.256 mmol), 4,4,5,5-tetramethyl-2-(perylene-3-yl)-1,3,2-dioxaborolane³ (0.097 g, 0.256 mmol), and Cs₂CO₃ (0.82 g, 2.5 mmol) were added to THF (50 mL) in a 2-neck round-bottom flask equipped with a water-jacketed reflux condenser. The solution was degassed (N_{2(g)}) for 15 minutes. Pd(PPh₃)₄ (0.035 g, 0.03 mmol) was added, and the solution was stirred at reflux under N_{2(g)} for 12 h. After cooling to room temperature, the solvent was removed by rotary evaporation, and the crude material was purified by column

chromatography on silica gel (25% DCM in hexanes) to give the product as a yellow powder (0.103 g, 76%). ¹H NMR (500 MHz, DMSO– d_6) δ 8.51–8.41 (m, 4H), 7.89–7.83 (m, 3H), 7.80 (d, J = 7.9 Hz, 2H), 7.64–7.56 (m, 6H), 7.17 (d, J = 7.6 Hz, 1H), 7.07 (dd, J = 7.9, 7.9 Hz, 1H), 6.95 (dd, J = 7.5, 7.5 Hz, 1H), 6.47 (d, J = 8.3 Hz, 1H). ¹³C NMR (126 MHz, DMSO– d_6) δ 143.7, 143.5, 141.8, 135.8, 133.4, 132.8, 130.2, 129.4, 129.0, 128.1, 127.7, 127.6, 125.2, 123.9, 121.9, 118.4, 117.5, 105.0. HRMS (ESI) m/z [M]⁺ calculated for C₃₈H₂₃NS 525.155, found 525.156.



PTZ-BE. 10-(4-bromophenyl)-10*H*-phenothiazine² (1.0 g, 2.82 mmol) bis(pinacolato)diboron (1.08 g, 4.23 mmol), and KOAc (0.46 g, 4.7 mmol) were added to 1,4-dioxane (70 mL) in a 2-neck round-bottom flask equipped with a water-jacketed reflux condenser. The solution was degassed (N_{2(g)}) for 15 minutes. Pd(dppf)Cl₂ (0.20 g, 0.15 mmol) was added, and the solution was stirred at 75 °C under N_{2(g)} for 12 h. After cooling to room temperature, the solvent was removed by rotary evaporation, and the crude material was purified by column chromatography on silica gel (DCM) to give the product as a white crystalline powder (0.91 g, 80%). ¹H NMR (500 MHz, DMSO–*d*₆) δ 7.88 (d, *J* = 8.3 Hz, 2H), 7.35 (d, *J* = 8.3 Hz, 2H), 7.18 (dd, *J* = 7.5, 1.6 Hz, 2H), 7.02 (ddd, *J* = 7.9, 7.7, 1.7 Hz, 2H), 6.95 (ddd, *J* = 7.5, 7.5, 1.3 Hz, 2H), 6.41 (dd, *J* = 8.1, 1.3 Hz, 2H), 1.33 (s, 12H). ¹³C NMR (126 MHz, DMSO–*d*₆) δ 144.5, 143.4, 137.3, 127.9, 127.6, 123.9,

122.4, 118.6, 84.3, 25.2. HRMS (ESI) m/z [M+H]⁺ calculated for C₂₄H₂₄BNO₂S 400.165, found 400.166.



PTZ-ACN. PTZ-BE (0.128 g, 0.319 mmol), 9-bromo-10-cyanoanthracene⁶ (0.060, 0.21 mmol), and Cs₂CO₃ (1.04 g, 3.2 mmol) were added to THF (20 mL) in a 2-neck round-bottom flask equipped with a water-jacketed reflux condenser. The solution was degassed (N_{2(g)}) for 15 minutes. Pd(PPh₃)₄ (0.023 g, 0.02 mmol) was added, and the solution was stirred at reflux under N_{2(g)} for 16 h. After cooling to room temperature, the solvent was removed by rotary evaporation, and the crude material was purified by column chromatography on silica gel (30% DCM in hexanes) to give the product as an orange powder (0.059 g, 58%). ¹H NMR (500 MHz, DMSO–*d*₆) δ 8.44 (d, *J* = 8.5 Hz, 2H), 7.93 (dd, *J* = 7.6, 7.6 Hz, 2H), 7.85 (d, *J* = 9.0 Hz, 2H), 7.76 – 7.61 (m, 6H), 7.23 (d, *J* = 7.5 Hz, 2H), 7.16 (dd, *J* = 7.9, 7.9 Hz, 2H), 7.01 (dd, *J* = 7.5, 7.5 Hz, 2H), 6.67 (d, *J* = 8.1 Hz, 2H). ¹³C NMR (126 MHz, DCM–*d*₂) 144.1, 143.0, 141.8, 136.5, 133.19, 133.17, 129.7, 129.4, 128.9, 127.8, 127.2, 127.1, 126.6, 125.6, 123.2, 122.2, 117.6, 117.3, 106.1. HRMS (ESI) *m*/*z* [M+H]⁺ calculated for C₃₃H₂₀N₂S 476.134, found 476.135.

2. Steady-State Optical Spectroscopy



Figure S1. Normalized steady-state absorption spectra of PTZ containing dyads (red) overlaid with their monomeric hole-accepting moieties (black).

3. Electrochemistry



Figure S2. Cyclic voltammograms of the PTZ containing dyads (solid line) compared with their monomeric hole accepting moieties.

4. Transient Absorption Spectroscopy

The data were globally fit either to specified kinetic models or a sum of exponentials. The dataset was then deconvoluted with the resultant populations or amplitudes to reconstruct the species-associated or decay-associated spectra. The kinetic data from multiple different wavelengths are fit using the global analysis described below. Each wavelength is given an initial amplitude that is representative of the spectral intensity at time t₀, and varied independently to fit the data. The time/rate constants and t₀ are shared between the various kinetic data and are varied globally across the kinetic data to fit the models described below.

For the species-associated fitting, we globally fit the dataset to a specified kinetic model (shown below each data set) and use the resultant populations to deconvolute the dataset and reconstruct species-associated spectra. The MATLAB program numerically the solves the differential equations through matrix methods, then convolutes the solutions with a Gaussian instrument response function with width w (FWHM), before employing a least-squares fitting using a Levenberg-Marquardt or Simplex method to find the parameters which result in matches to the kinetic data.

For decay-associated fitting, we globally fit the dataset to a set of pre-specified mathematical functions and use the resultant function amplitudes to deconvolute the dataset and reconstruct decay-associated spectra:

$$S(\lambda, t) = \sum_{n} A_{n}(\lambda, 0) \exp\left[-t/\tau_{n}\right]$$
 (Eqn. S1)

The MATLAB program convolutes the solutions with a Gaussian instrument response function with width w (FWHM), before employing a least-squares fitting using a Levenberg-Marquardt or Simplex method to find the parameters which result in matches to the kinetic data. Each function corresponds to a given well-defined temporal process. The raw data matrix is deconvoluted with the resultant function amplitudes as functions of time to produce the spectra associated with each mathematical component, $A_n(\lambda)$.

The time constants extracted from the fits of the fsTA data and summarized in Table 2 of the main text are effective time constants (τ_{eff}) and may be combinations of multiple photophysical processes. The effective time constants were used to determine time constants for each individual photophysical pathway to the best of our ability (displayed in Figure 8 of the main text) using Equation S2.

$$\frac{1}{\tau_{eff}} = \frac{1}{\tau_1} + \frac{1}{\tau_2} + \dots + \frac{1}{\tau_n}$$
(Eqn. S2)



Figure S3. $\lambda_{ex} = 517$ nm, 1.0 µJ/pulse, MeCN. (A) fsTA spectra of PTZ⁺⁺. (B) Species-associated spectra obtained by global fitting. (C) Transient kinetics at selected wavelengths. (D) Populations of the transient species. (E) fsTA spectra of PTZ⁺⁺ expanded to show the evolution in ESA wavelength of maximum intensity over the first 100 ps.

$$k = \begin{bmatrix} -k_{A \to B} & 0 \\ k_{A \to B} & -k_{B \to GS} \end{bmatrix}$$

Initial populations: $A_0 = 1$ and $B_0 = 0$

Following excitation at $\lambda = 517$ nm, PTZ⁺⁺ exhibits a strong excited state absorption (ESA) at $\lambda = 380$ nm, a ground state bleach (GSB) at $\lambda = 514$ nm, and a weak ESA at $\lambda = 568$ nm. Each of these signals is apparent after a 1 ps delay. The weaker ESA undergoes a hypsochromic shift from $\lambda = 568$ to 548 nm as the spectra evolve over the first 50 ps (Figure S3E). The stronger ESA concomitantly undergoes a less dramatic shift from $\lambda = 380$ to 374 nm. This dynamic spectral shifting is indicative of a GS recovery mechanism composed of multiple species, and this mechanism is supported by the global fitting analysis (Figure S3). Following excitation at $\lambda = 900$ nm, the ESA features at $\lambda = 380$ and 568 nm and GSB at $\lambda = 514$ nm are again apparent after a 1 ps delay, and again the ESA features again shift to $\lambda = 374$ and 548 nm as the spectra evolve over the first 50 ps (Figure S5).



Figure S4. $\lambda_{ex} = 517$ nm, 1.0 µJ/pulse, MeCN. (A) NIR fsTA spectra of PTZ⁺⁺. (B) Species-associated spectra obtained by global fitting. (C) Transient kinetics at selected wavelengths. (D) Populations of the transient species.

$$k = \begin{bmatrix} -k_{A \to B} & 0 \\ k_{A \to B} & -k_{B \to GS} \end{bmatrix}$$

Initial populations: $A_0 = 1$ and $B_0 = 0$



Figure S5. $\lambda_{ex} = 900$ nm, 1.0 µJ/pulse, MeCN. (A) fsTA spectra of PTZ⁺⁺. (B) Species-associated spectra obtained by global fitting. (C) Transient kinetics at selected wavelengths. (D) Populations of the transient species. (E) fsTA spectra of PTZ⁺⁺ expanded to show the evolution in ESA wavelength of maximum intensity over the first 100 ps.

$$k = \begin{bmatrix} -k_{A \to B} & 0 \\ k_{A \to B} & -k_{B \to GS} \end{bmatrix}$$

Initial populations: $A_0 = 1$ and $B_0 = 0$



Figure S6. $\lambda_{ex} = 900$ nm, 1.0 µJ/pulse, MeCN. (A) NIR fsTA spectra of PTZ⁺⁺. (B) Species-associated spectra obtained by global fitting. (C) Transient kinetics at selected wavelengths. (D) Populations of the transient species.

$$k = \begin{bmatrix} -k_{A \to B} & 0 \\ k_{A \to B} & -k_{B \to GS} \end{bmatrix}$$

Initial populations: $A_0 = 1$ and $B_0 = 0$



Figure S7. $\lambda_{ex} = 517$ nm, 1.0 µJ/pulse, MeCN. (A) fsTA spectra of PTZ⁺⁻-Per. (B) Species-associated spectra obtained by global fitting. (C) Transient kinetics at selected wavelengths. (D) Populations of the transient species.

$$\boldsymbol{k} = \begin{bmatrix} -\boldsymbol{k}_{A \to GS} & \boldsymbol{0} \\ \boldsymbol{0} & -\boldsymbol{k}_{B \to GS} \end{bmatrix}$$

Initial populations: $A_0 = 0.86$ and $B_0 = 0.14$

After a delay of 0.7 ps following excitation of PTZ^{+*}-Per with a pump pulse centered at $\lambda_{ex} = 517$ nm, an absorptive feature at $\lambda = 565$ nm, characteristic of Per^{+*}, and Per GSB features at $\lambda = 416$ and 442 nm are apparent (Figure 4A).⁸ These features reach maximum intensity at a pump-probe delay of 1.7 ps, after which they begin to decay. Because the PTZ^{+*} GS NIR absorption band is significantly less intense than the GS visible absorption band (Figure 1B) the samples prepared for excitation at $\lambda_{ex} = 900$ nm were more concentrated than those prepared for $\lambda_{ex} = 517$ nm. This

resulted in the Per GS completely absorbing the light from the probe pulse between $\lambda = 405$ and 450 nm, thus no data were recorded in this region.

The GS recovery dynamics of PTZ⁺⁺-Per were observed to be biexponential after excitation at $\lambda_{ex} = 517$ nm. This is explained by structural relaxation of neutral PTZ moiety after the initial hole transfer reaction (main text). To determine the percentage of the population that decays to the GS from each Species A and Species B, the initial populations were adjusted until the magnitude of the Per GSB was equivalent for both species (Figure S7B). It was determined that 86% of the sample decays back to the ground state through Species A, and 14% of the sample decays to the ground state through Species B. From this, the time constant for the structural relaxation of the neutral PTZ moiety was estimated to be ~270 ps. Using this value, a new rate matrix was used to fit the data to a model that more accurately represents the photophysical dynamics (Figure S8). This same matrix was also used to fit the data collected after excitation at $\lambda_{ex} = 900$ nm (Figure S10).



Figure S8. $\lambda_{ex} = 517$ nm, 1.0 µJ/pulse, MeCN. (A) fsTA spectra of PTZ⁺⁺-Per. (B) Species-associated spectra obtained by global fitting. (C) Transient kinetics at selected wavelengths. (D) Populations of the transient species.

$$k = \begin{bmatrix} -k_{A \to GS} - \left(\frac{1}{270}\right) & \mathbf{0} \\ \left(\frac{1}{270}\right) & -k_{B \to GS} \end{bmatrix}$$

Initial populations: $A_0 = 1$ and $B_0 = 0$



Figure S9. $\lambda_{ex} = 900$ nm, 1.0 µJ/pulse, MeCN. (A) fsTA spectra of PTZ⁺⁻-Per. (B) Species-associated spectra obtained by global fitting. (C) Transient kinetics at selected wavelengths. (D) Populations of the transient species.

$$\boldsymbol{k} = \begin{bmatrix} -\boldsymbol{k}_{A \to GS} & \boldsymbol{0} \\ \boldsymbol{0} & -\boldsymbol{k}_{B \to GS} \end{bmatrix}$$

Initial populations: $A_0 = 0.86$ and $B_0 = 0.14$



Figure S10. $\lambda_{ex} = 900$ nm, 1.0 µJ/pulse, MeCN. (A) fsTA spectra of PTZ⁺⁺-Per. (B) Species-associated spectra obtained by global fitting. (C) Transient kinetics at selected wavelengths. (D) Populations of the transient species.

$$\boldsymbol{k} = \begin{bmatrix} -\boldsymbol{k}_{A \to GS} - \left(\frac{1}{270}\right) & \boldsymbol{0} \\ \left(\frac{1}{270}\right) & -\boldsymbol{k}_{B \to GS} \end{bmatrix}$$

Initial populations: $A_0 = 1$ and $B_0 = 0$



Figure S11. $\lambda_{ex} = 517$ nm, 1.0 µJ/pulse, MeCN. (A) fsTA spectra of PTZ⁺⁻DPA. (B) Decay-associated spectra obtained by global fitting. (C) Transient kinetics at selected wavelengths. (D) Amplitudes of the exponential functions used in the fitting.

$$A(t) = A_0 \exp\left[-\frac{t}{t_1}\right]$$
$$B(t) = B_0 \exp\left[-\frac{t}{t_2}\right]$$
$$C(t) = C_0 \exp\left[-\frac{t}{t_{13}}\right]$$

After a delay of 0.5 ps following excitation of PTZ⁺-DPA at $\lambda_{ex} = 517$ nm, features at $\lambda = 417$, 589, and 654 nm characteristic of DPA⁺ are apparent (Figures 5A and S11A).⁹⁻¹⁰ At delays longer than 2 ps, an absorptive feature is apparent at $\lambda = 548$ nm. The decay-associated spectrum with the

shortest time constant (component A in Figures 5B and S11B) has features characteristic of the PTZ⁺⁺ GSB and decays with $\tau_A = 0.9 \pm 0.3$ ps. Component B in Figure 5B has features at $\lambda = 417$, 589, and 654 nm, characteristic of DPA⁺⁺, and this component decays with a time constant of $\tau_B = 4.1 \pm 0.3$ ps. Component C is the decay of the feature at $\lambda = 548$ nm, and it decays with a time constant of $\tau_C = 20 \pm 2$ ps. Following excitation at $\lambda_{ex} = 900$ nm features assigned to DPA⁺⁺ and the PTZ⁺⁺ GSB are again apparent after a delay of 0.5 ps. Unlike the spectra following $\lambda_{ex} = 517$ nm excitation, when the sample is excited at $\lambda_{ex} = 900$ nm the feature at $\lambda = 548$ nm is not significant at longer time delays (Figures 5C and S12A).



Figure S12. $\lambda_{ex} = 900$ nm, 1.0 µJ/pulse, MeCN. (A) fsTA spectra of PTZ⁺-DPA. (B) Decay-associated spectra obtained by global fitting. (C) Transient kinetics at selected wavelengths. (D) Amplitudes of the exponential functions used in the fitting.

$$A(t) = A_0 \exp\left[-\frac{t}{t_1}\right]$$
$$B(t) = B_0 \exp\left[-\frac{t}{t_2}\right]$$



Figure S13. (A) NIR probe fsTA spectra of PTZ⁺⁺-DPA $\lambda_{ex} = 517$ nm, 1.0 µJ/pulse, MeCN. (B) NIR probe fsTA spectra of PTZ⁺⁺-DPA $\lambda_{ex} = 900$ nm, 1.0 µJ/pulse, MeCN.



Figure S14. $\lambda_{ex} = 517$ nm, 1.0 µJ/pulse, MeCN. (A) fsTA spectra of PTZ⁺⁻ACN. (B) Species-associated spectra obtained by global fitting. (C) Transient kinetics at selected wavelengths. (D) Populations of the transient species.

$$k = \begin{bmatrix} -\mathbf{k}_{A \to B} & 0 & 0 \\ \mathbf{k}_{A \to B} & -\mathbf{k}_{B \to GS} & 0 \\ 0 & 0 & -\mathbf{k}_{C \to GS} \end{bmatrix}$$

Initial populations: $A_0 = 1$, $B_0 = 0$, and $C_0 = 1$

Following excitation of PTZ^{+} -ACN at $\lambda_{ex} = 517$ nm, a broad absorptive feature between $\lambda = 600$ and 700 nm, the region, where oxidized anthracenes typically absorb,⁹ is apparent after a delay of 0.6 ps (Figures 6A and S14A). This feature decays rapidly and a feature resembling the ²*PTZ⁺ ESA remains, which then undergoes a hypsochromic shift before decaying completely by a delay of 60 ps (Figure 6A and S14A). When the sample was irradiated with a $\lambda_{ex} = 900$ nm excitation

pulse, PTZ^{+} GSB and ESA are apparent after a 0.6 ps delay, but no broad feature between $\lambda = 600$ and 700 nm is observed (Figures 6C and S15A). The ²*PTZ+• ESA undergoes the usual hypsochromic shift before decaying completely. No broad anthracene feature between $\lambda = 600$ and 700 nm is observed.



Figure S15. $\lambda_{ex} = 900$ nm, 1.0 µJ/pulse, MeCN. (A) fsTA spectra of PTZ⁺⁻ACN. (B) Species-associated spectra obtained by global fitting. (C) Transient kinetics at selected wavelengths. (D) Populations of the transient species.

$$k = \begin{bmatrix} -\mathbf{k}_{A \to GS} & 0 \\ \mathbf{k}_{A \to B} & -\mathbf{k}_{B \to GS} \end{bmatrix}$$

Initial populations:
$$A_0 = 1$$
 and $B_0 = 0$



Figure S16. (A) NIR probe fsTA spectra of PTZ⁺⁺-ACN $\lambda_{ex} = 517$ nm, 1.0 µJ/pulse, MeCN. (B) NIR probe fsTA spectra of PTZ⁺⁺-DPA $\lambda_{ex} = 900$ nm, 1.0 µJ/pulse, MeCN..

5. Raman Spectroscopy



Figure S17. (A) Steady-state FSRS spectrum of a solution of PTZ^{+} in MeCN (*d*-3) obtained with a 540 nm (~1 ps, 0.7 μ J) Raman pump. (B) Computed normal modes.

The steady-state FSRS spectrum collected with Raman pump centered at $\lambda_{RP} = 540$ nm provides the resonance Raman spectrum for the PTZ^{*+} D₀ state and shows multiple features from 200-700 cm⁻¹ and 1000-1600 cm⁻¹ (Figure S15A). It is reproduced reasonably well by the normal mode analysis (Figure S15B) and is consistent with previously reported time-resolved resonance Raman spectra.¹¹ The calculated PTZ^{+*} spectrum was optimized in Gaussian 09 at CAMB3LYP/ 6-311+G(d,p) level of theory with tight convergence criteria on the forces and step sizes. Taking the optimized geometry, the Raman spectrum was computed at the same level of theory. The computed frequencies were scaled by an empirical factor of 0.951.¹² The intensities in both the experimental and computed Raman spectra (Figure S15) have been normalized for a clearer comparison.

Addition of an actinic pump at $\lambda = 515$ nm promotes a portion of the sample to an excited electronic state, which is subsequently probed with $\lambda_{RP} = 400$ nm to collect the resonance Raman spectrum of the excited electronic state at various time delays (Figure S16A). A single weak transient feature is observed at 1346 cm⁻¹ upon excitation and no new features appear as it decays. The 1346 cm⁻¹ feature likely represents a normal mode similar to the calculated 1290 cm⁻¹ ring deformation mode (Figure S16B). Both the amplitude and the numerical area of the 1346 cm⁻¹ feature were found to decay monoexponentially with $\tau \sim 35$ ps (Figure S16C-E). These observations suggest that the transient population is decaying from the electronic excited state back to the electronic ground state with $\tau \sim 35$ ps. Additionally, the centroid of the 1346 cm⁻¹ feature appears to undergo a small shift to higher frequencies around $\Delta t \sim 10$ ps (Figure S16F). This shift is consistent with the fast process observed in the fsTA experiment representing relaxation along the excited electronic potential energy surface.



Figure S18. $\lambda_{ex} = 515 \text{ nm} (<100 \text{ fs}, 1 \text{ µJ}), \lambda_{RP} = 400 \text{ nm} (~1 \text{ ps}, 0.7 \text{ µJ}), CD_3CN (A) Time-resolved FSRS spectra of PTZ⁺⁺. (B) Nearest calculated mode in D₀. (C) Decay-associated spectra and (D) kinetics overlaid with fit following SVD analysis and global fitting to an exponential decay convoluted with a Gaussian instrument response. (E) Numerical area for 1300-1390 cm⁻¹ overlaid with fit to the sum of an exponential decay and a step function convoluted with a Gaussian instrument response. (F) Centroid for 1300-1390 cm⁻¹.$

Raman Frequency (cm ⁻¹)		Mada Displacement	
Experiment	Computation	- Mode Displacement	
291	446		
375	517		
501	588		
668	762		
1045	1120		
1103	1156		

Table S1. Experimental and Computational Raman Frequencies and mode displacements.

1261	1193	
1299	1236	
1348	1290	
1484	1429	
1586	1569	

6. Computational Section

Coordinates of optimized PTZ^{+•}

С	-7.62215900	-3.65967500	0.13553800
С	-6.51910800	-3.46843500	-0.69148600
С	-5.83402900	-2.24382200	-0.67287900

С	-6.30559800	-1.18885000	0.14335700
С	-7.38584000	-1.41416000	1.01538100
С	-8.03706300	-2.64242700	1.00904500
С	-4.22861700	0.02499300	0.16494800
С	-3.52490900	-0.90004300	-0.64160100
С	-2.12160000	-0.90504400	-0.62991900
Н	-1.57804600	-1.61025900	-1.26261300
С	-1.43177600	-0.04125500	0.21612500
С	-2.13202400	0.82062800	1.07514100
С	-3.52113100	0.85783000	1.05109400
Н	-8.14061800	-4.62102200	0.12795100
Н	-6.16114100	-4.27780900	-1.33153600
Н	-7.69380800	-0.62779900	1.70529800
Н	-8.86718000	-2.81390800	1.69751900
Н	-0.33977900	-0.06295100	0.23295700
Н	-1.58905300	1.45977000	1.77458000
Н	-4.07083200	1.51650500	1.72477900
Ν	-5.64853900	0.07365900	0.07538500
S	-4.39022400	-2.04530400	-1.66715700
С	-6.33604100	1.26878700	-0.17214000
С	-5.62467700	2.48367600	-0.38789000
С	-7.75374900	1.28916000	-0.30044500
С	-6.30887500	3.66378900	-0.64056600

Η	-4.53770700	2.50204200	-0.38866600
С	-8.41881900	2.48015900	-0.55322000
Н	-8.33585800	0.37476700	-0.22484000
С	-7.70937600	3.67999100	-0.70869800
Н	-5.74065400	4.58206600	-0.80409800
Н	-9.50709400	2.47045400	-0.64471400
Н	-8.24117500	4.61290400	-0.90879200

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