

Supporting Information

Investigation of Strain-Promoted Azide-Alkyne Cycloadditions in Aqueous Solutions by Capillary Electrophoresis

Jana Steflova,^{,†,‡} Golo Storch,[†] Sarah Wiesner,[†] Skrollan Stockinger,[†] Regina Berg[†] and Oliver Trapp^{*,†}*

[†]Department Chemie, Ludwig-Maximilians-Universität München,

Butenandtstr. 5–13, 81377 München, Germany

oliver.trapp@cup.uni-muenchen.de

[‡]Charles University, Faculty of Science, Department of Physical and Macromolecular Chemistry, Hlavova

8, 128 40 Prague 2, Czech Republic

svobod.j@natur.cuni.cz

Content

1	Electrophoretic Method and Experimental Conditions.....	S6
1.1	Offline Reaction Method.....	S6
1.2	Kinetics of Second Order Reactions.....	S6
1.3	Method Evaluation.....	S7
1.4	Conditions of Simulations.....	S9
2	Synthesis of Azides.....	S10
2.1	Preparation of Phenyl Azide.....	S10
2.2	General Procedure Azidation.....	S10
2.3	Preparation of p-Azidobenzoic Acid.....	S10
2.4	Preparation of p-Azidophenol.....	S10
2.5	Preparation of Sodium p-Azidobenzenesulfonate.....	S10
3	Determination of pKa Values of Reactants and Selected Products.....	S11
4	DFT Calculations.....	S20
4.1	Ground State Optimization.....	S20
4.2	Non-Protonated (NH ₂) Cyclooctyne.....	S20
4.2.1	Amide E-Isomer.....	S20
4.2.2	Amide Z-Isomer.....	S21
4.3	Protonated (NH ₃ ⁺) Cyclooctyne	S21
4.4	Phenyl Azide.....	S22
4.5	Methyl Azide.....	S22
5	Phenyl Azide (PhN ₃) Transition States.....	S22
5.1	Non-Protonated (NH ₂) Cyclooctyne.....	S22
5.2	Protonated (NH ₃ ⁺) Cyclooctyne.....	S23
6	Methyl Azide (MeN ₃) Transition States.....	S24
6.1	Non-Protonated (NH ₂) Cyclooctyne.....	S24

6.2	Protonated (NH_3^+) Cyclooctyne.....	S24
7	Coordinates of Ground States.....	S25
7.1	Non-Protonated (NH_2) Cyclooctyne.....	S25
7.1.1	E-1 _{sp} -2P _{sc}	S25
7.1.2	E-1 _{sp} -2M _{sc}	S25
7.1.3	E-1 _{sp} -2 _{ap}	S26
7.1.4	E-1P-2P _{sc}	S27
7.1.5	E-1P-2M _{sc}	S27
7.1.6	E-1P-2 _{ap}	S28
7.1.7	E-1M-2P _{sc}	S29
7.1.8	E-1M-2M _{sc}	S30
7.1.9	E-1M-2 _{ap}	S30
7.1.10	Z-1 _{sp} -2P _{sc}	S31
7.1.11	Z-1 _{sp} -2M _{sc}	S32
7.1.12	Z-1 _{sp} -2 _{ap}	S33
7.1.13	Z-1P-2P _{sc}	S33
7.1.14	Z-1P-2M _{sc}	S34
7.1.15	Z-1P-2 _{ap}	S35
7.1.16	Z-1M-2P _{sc}	S35
7.1.17	Z-1M-2M _{sc}	S36
7.1.18	Z-1M-2 _{ap}	S37
7.1.19	E-1M-2M _{sc} (water)	S38
7.2	Protonated (NH_3^+) Cyclooctyne.....	S38
7.2.1	E-1 _{sp} -2P _{sc}	S38
7.2.2	E-1 _{sp} -2M _{sc}	S39
7.2.3	E-1 _{sp} -2 _{ap}	S40

7.2.4	E-1P-2 _{ap}	S40
7.2.5	E-1M-2P _{sc}	S41
7.2.6	E-1M-2M _{sc}	S42
7.2.7	E-1M-2 _{ap}	S43
7.2.8	Z-1 _{sp} -2P _{sc}	S43
7.2.9	Z-1 _{sp} -2M _{sc}	S44
7.2.10	E-1 _{sp} -2P _{sc} (water)	S45
7.3	Azides.....	S46
7.3.1	Phenyl Azide (MeCN)	S46
7.3.2	Phenyl Azide (water)	S46
7.3.3	Methyl Azide (MeCN)	S46
8	Coordinates of Transition States.....	S47
8.1	Phenyl Azide (PhN ₃) ⁺ Non-Protonated Cyclooctyne.....	S47
8.1.1	E-1M-2M _{sc} -anti-11.....	S47
8.1.2	E-1M-2M _{sc} -syn-11.....	S48
8.1.3	E-1M-2M _{sc} -syn-12.....	S49
8.1.4	Z-1 _{sp} -2M _{sc} -syn-12.....	S49
8.1.5	E-1M-2M _{sc} -syn-12 (water)	S50
8.2	Phenyl Azide (PhN ₃) ⁺ Protonated Cyclooctyne.....	S51
8.2.1	E-1 _{sp} -2P _{sc} -anti-11.....	S51
8.2.2	E-1 _{sp} -2P _{sc} -syn-11.....	S52
8.2.3	E-1 _{sp} -2P _{sc} -syn-12.....	S53
8.2.4	Z-1 _{sp} -2P _{sc} -anti-11.....	S54
8.2.5	E-1 _{sp} -2M _{sc} -syn-11.....	S55
8.2.6	E-1 _{sp} -2P _{sc} -anti-11 (water)	S56
8.2.7	E-1 _{sp} -2M _{sc} -syn-11 (water)	S57

8.3	Methyl Azide (MeN_3) ⁺ Non-Protonated (NH_2) alkyne.....	S58
8.3.1	E-1M-2M _{sc} -syn-12.....	S58
8.3.2	E-1M-2M _{sc} -anti-11.....	S59
8.4	Methyl Azide (MeN_3) ⁺ Protonated (NH_3^+) alkyne.....	S60
8.4.1	E-1 _{sp} -2P _{sc} -syn-12.....	S60
8.4.2	E-1 _{sp} -2P _{sc} -anti-11.....	S61
9	Characterization of Interaction of Individual Reactants with SDS by Investigating the Effect on Effective Mobility.....	S63
10	Determination of the Critical Micelle Concentration (CMC).....	S64
10.1	FCS Measurements.....	S64
10.2	Mobility Measurements.....	S64
11	NMR Spectra.....	S66
11.1	Phenyl Azide.....	S66
11.2	p-Azidobenzoic Acid.....	S67
11.3	Sodium p-Azidobenzenesulfonate.....	S68
11.4	p-Azidophenol.....	S69
12	References.....	S70

1 Electrophoretic Method and Experimental Conditions

1.1 Offline Reaction Method

Table SI-1 Composition, concentrations of the constituents (*c*), experimental pH and theoretical pH calculated by PeakMaster 5.3 software of the running buffers for rate constant determination.

Buffer constituents	SDS	Maleic a. /LiOH	Citric a. /LiOH	Phosphoric a. /NaOH	β-Alanine /LiOH
<i>c</i> / mM		13 / 5.5	15 / 10	12 / 15	7 / 10
IS / mM		9.97	10.0	18.0	9.96
pH H ₂ O/MeCN	0	2.29	3.77	7.09	11.55
	20	1.97	3.42	6.59	11.45
	50	1.95	3.35	6.39	11.39
pH H ₂ O	0	2.39	3.37	6.73	11.49
	20	2.56	3.39	6.45	11.45
	50	2.78	3.40	6.44	11.44
pH theor	0	2.39	3.36	6.57	11.45

1.2 Kinetics of Second Order Reactions

The rate of the strain-promoted cycloaddition of cyclooctyne and azide is first order in each of the reactants. Thus, the overall reaction is second order and the reaction rate is defined as

$$-\frac{d[A]}{dt} = k[A][B], \quad (1)$$

where [A] and [B] are the equilibrium concentrations of the reactants and *k* is the corresponding rate constant. This differential equation can be solved for two particular cases:

The initial concentrations of the reactants is the same, then

$$\frac{1}{c_A} = \frac{1}{c_A^0} + 2kt, \quad (2)$$

where c_A^0 is the initial concentrations of both reactants.

The initial concentrations of reactants differ, then

If the initial concentrations of reactants differ, then

$$\frac{c_A}{c_B} = \frac{c_A^0}{c_B^0} e^{(c_A^0 - c_B^0)kt}, \quad (3)$$

where c_B^0 , c_A^0 are the initial concentrations of the reactants.

The area of separated peaks of reactants in CZE is directly proportional to their respective concentration in the mixture. Thus, equation (3) can be further transformed to the following form

$$\frac{A_A}{A_B} = \frac{A_A^0}{A_B^0} e^{(c_A^0 - c_B^0)kt}, \quad (4)$$

where A_A^0 and A_B^0 are initial areas of reactant peaks and A_A and A_B are peak areas at time t .

The equation can be further linearized for better visualization of the quality of the data

$$\ln \frac{A_B}{A_A} = \ln \frac{A_B^0}{A_A^0} + (c_B^0 - c_A^0)kt, \quad (5)$$

The second approach was selected for this study. Advantageously, as there are no degradation pathways or side reactions, only the ratio of the two reactants' peak areas in dependence on time t is necessary to investigate the kinetics of this reaction, the absolute concentrations themselves are not required. Thus, no internal standard or calibration is needed.

The slope of the function $\ln \frac{A_B}{A_A}(t)$ is the product of the difference of initial concentrations ($c_B^0 - c_A^0$) and the rate constant k , thus the slope of this function can be directly influenced by changing the initial concentrations of reactants, which enhances the applicability of this method for a wide range of rate constants.

1.3 Method Evaluation

The rate constants were determined by CZE. The offline reactions were run directly in the electrophoretic vial and the reaction mixture was continuously analyzed by CZE with UV detection. The areas of reactant peaks were integrated by the ChemStation program, the time dependence of the natural logarithm of the area ratio of the azide and DBCO-amine peaks was evaluated according to Eq.6. The injection time was considered as time when the reaction was interrupted. An example of the obtained electropherograms and their evaluation is shown in Figure 1B, 1C, respectively.

It has to be noted that it takes a certain amount of time for the zones of reactants to separate and during this time the reaction proceeds. The impact of this additional online reaction during the separation procedure on the area ratio of the reactants and consequently on the rate constant was modelled by dynamic simulations using the program Simul 5 Complex-Kinetic. Simulations were performed on a workstation equipped with Intel® Core™ i5-3470 CPU 3.20 GHz. The simulation time was in the range of hours.

Applying Simul 5 Complex-Kinetic, it is possible to simulate the electrophoretic separation for systems with complexation equilibria involved. Consequently, these simulations can also be adapted for simulating the influence of reversible on-column reactions, whose rate is first or second order.

The kinetic model of Simul 5 Complex-Kinetic was confirmed by the following test: the capillary was filled with the initial composition of the reaction mixture (DBCO-amine 0.5 mM, azide 1 mM), the rate constant of the forward reaction was set as $12 \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}$ and the rate constant of the reverse reaction was set 10^7 times lower ($12 \cdot 10^{-7} \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}$). The voltage was set to 0 kV and no diffusion was applied. The concentration of reactants was monitored over time and the rate constant was calculated according to Eq. 3. The resulting rate constant exactly matched the input value.

In the next step, separation of the initial reaction mixture was simulated. The simulations were performed for reaction rates ranging from $0 \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}$ to $30 \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}$. Exemplifying electropherograms for $12 \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}$ and $0 \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}$ are shown in Figure SI-1.

It is obvious that only a very small amount of the product was formed during the online reaction, and the change in the natural logarithm of area ratios was always lower than 4 %, even at the highest reaction rate ($12 \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}$). This error can be neglected in comparison with the errors caused by integration of separated peaks and thus the on-column reaction progress was not considered in our kinetic analysis.

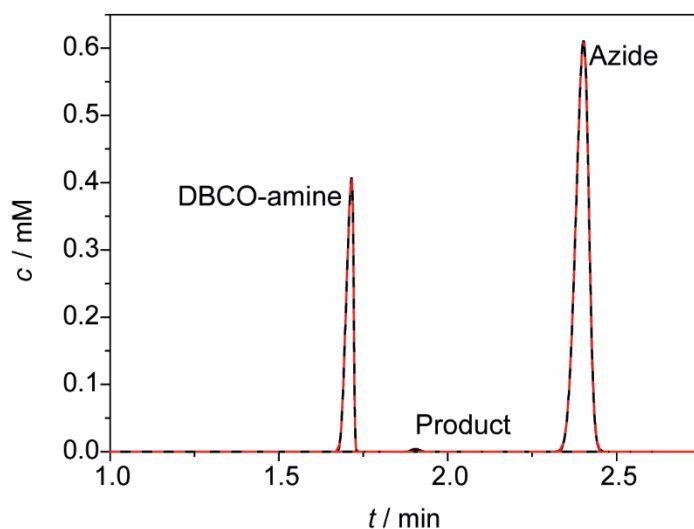


Figure SI-1 Simulated electropherograms of initial DBCO-amine reaction mixture of Phe-N₃ with DBCO-amine calculated by Simul 5 Complex-Kinetic. Black solid line: online reaction simulated with a forward reaction rate constant of $12 \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}$, backward rate constant $12 \cdot 10^{-7} \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}$; Red dashed lines: online reaction not considered. Initial concentration of cyclooctyne and azide was 1.0 and 0.5 mM, respectively.

1.4 Conditions of Simulations

The experimental conditions used for simulations were adapted in order to minimize the simulation time. A capillary of 10 % of the original capillary's length was used (35.9 mm), and the decrease in capillary length compensated by lowering the voltage by factor 100 (200 V). The injection site was at 3 mm and the detector was situated at 30.4 mm. Simultaneously, the length of injected zones was reduced to 0.325 mm, peak edge 0.1625 mm. This setup leads to significant reduction of simulation time.

The capillary was filled with 7 mM β -AL/10 mM LiOH buffer. The analyte zones contained 1 mM azide and 0.5 mM DBCO-amine in 7 mM β -AL/10 mM LiOH buffer. Limiting mobilities and pK_a values at current ionic strength of reactants are shown in Table SI-2.

Reaction rate varied from 0 to $0.3 \text{ mol dm}^{-3}\text{s}^{-1}$. The mobility of EOF was set the same as during the corresponding experiment, $54.6 \cdot 10^{-9} \text{ m}^2\text{s}^{-1}\text{V}^{-1}$. The number of nodes on x axes was 20 000.

2 Synthesis of Azides

2.1 Preparation of Phenyl Azide

Phenyl azide was synthesized starting with phenyl hydrazine based on the procedure of Nguyen and Miles.¹ The ¹H NMR spectrum was in accordance with the data reported in literature. ¹H NMR (500 MHz, CDCl₃) δ = 7.41–7.31 (m, 2 H), 7.19–7.10 (t, *J* = 7.4 Hz, 1 H), 7.28 (d, *J* = 7.7 Hz, 2 H) ppm.

2.2 General Procedure Azidation

According to the work of Emrick *et al.*,² an aqueous solution of sodium nitrite (1.25 equiv.) was added dropwise to a solution of the amine (1.00 equiv.) in 2 N hydrochloric acid (20 mL) with ice cooling. After an hour, an aqueous solution of sodium azide (2.00 equiv.) was added and stirred at room temperature for at least 15 hours. Purification procedures for the different azide products are detailed below.

2.3 Preparation of *p*-Azidobenzoic Acid

p-Aminobenzoic acid (1.00 g, 7.29 mmol), NaNO₂ (629 mg, 9.11 mmol) and NaN₃ (948 mg, 14.6 mmol) were reacted according to the general procedure (*vide supra*). In analogy to the work of Poláková *et al.*,³ the reaction mixture was purified by pouring it into ice cold water, filtering off, washing with water and drying under reduced pressure. The desired product was obtained in 68 % yield (808 mg, 4.95 mmol). ¹H NMR (500 MHz, *d*₆-DMSO) δ = 14.47–11.30 (s, br, 1H), 7.95 (d, *J*=8.1 Hz, 2H), 7.20 (d, *J* = 8.1 Hz, 2H) ppm; ¹³C{¹H} NMR (126 MHz, *d*₆-DMSO) δ 166.6, 144.0, 131.3, 127.3, 119.2 ppm.

2.4 Preparation of *p*-Azidophenol

This compound was prepared according to a procedure from literature.² *p*-Aminophenol (5.00 g, 45.8 mmol), NaNO₂ (3.79 g, 54.9 mmol) and NaN₃ (4.50 g, 69.0 mmol) were reacted according to the general procedure (*vide supra*). For purification the mixture was extracted with ethyl acetate, the combined organic layers were washed with water and dried over MgSO₄. After filtration of the drying agent, the solvent was removed under reduced pressure. The residue was purified by column chromatography (hexane/ethyl acetate, 5/1) to obtain the desired product in 67 % yield (4.99 g, 37.0 mmol). ¹H NMR (500 MHz, CD₂Cl₂) δ 6.98–6.88 (m, 2H), 6.87–6.78 (m, 2H), 5.05 (s, br, 1H) ppm; ¹³C{¹H} NMR (126 MHz, CD₂Cl₂) δ 153.5, 133.0, 120.7, 117.1 ppm.

2.5 Preparation of Sodium *p*-Azidobenzenesulfonate

This compound was prepared using a modified literature procedure.^{3,4} An aqueous solution of NaNO₂ (497 mg, 7.22 mmol) was added dropwise to a solution of sulfanilic acid (1.00 g, 5.77 mmol) in 2 N

hydrochloric acid (20 mL) under ice cooling. After an hour, an aqueous solution (3 mL) of sodium azide (2.00 equiv.) was added and stirred at room temperature for at least 15 hours. The solid sodium salt was formed by adding sodium chloride, separated by filtration and dried under reduced pressure. Sodium *p*-azidobenzenesulfonate was obtained in 56 % yield (711 mg, 3.21 mmol), including approximately 10 % sodium chloride according to elemental analysis. ¹H NMR (400 MHz, *d*₆-DMSO) δ 7.64 (d, *J* = 8.5 Hz, 1H), 7.08 (d, *J* = 8.5 Hz, 1H) ppm; ¹³C{¹H} NMR (101 MHz, *d*₆-DMSO) δ 145.0, 139.5, 127.5, 118.4 ppm; elemental analysis: calculated C – 32.58 %, H – 1.82 %, N – 19.00 %, S – 14.50 %, Na – 10.39 %, O – 21.70 %; found: C – 29.40 %, H – 1.91 %, N – 17.31 %, Cl – 7.82 %.

3 Determination of pK_a Values of Reactants and Selected Products

Dissociation constants of all reactants were first predicted theoretically using Marvin Sketch 6.0.0 software. Based on this data, we proposed a set of separation buffers to cover a sufficient range of pH values using PeakMaster 5.3. The ionic strength was kept constant at 10 mM. The composition and characteristics of the employed buffers are summarized in Table SI-2.

The slight disagreement between the pH of buffers predicted by the PeakMaster software and measured values is connected to the presence of MeCN. Thus, the calculated values of pK_a are valid only for solutions containing 28 vol% MeCN.

The samples were injected hydrodynamically at 30 mbar×5s. The concentration of analytes was 2 mM, DMSO 0.2 vol%. was used as EOF marker. The voltage applied was 20 kV. In the acidic pH region, a hydrodynamic pressure of 50 mbar was applied. The measurements were performed at a constant temperature of 20°C.

The capillaries were flushed for 3 min with the respective buffer before every measurement. All measurements were performed in triplicates. Dissociation constants of all reactants and selected isomeric products of the reaction of PhOH-N₃ were determined in order to be able to discuss the influence of pH, and consequently dissociation (protonation) of reactants, on the rate of reaction. The dissociation constants were determined based on the dependence of the effective mobility of each compound on the pH value of the buffer. Obtained dependences were fitted by the following equations

$$u_{eff} = \frac{u_C^0}{1 + 10^{(pH-pKa)}}, \quad (5)$$

$$u_{eff} = \frac{u_A^0}{1 + 10^{(pKa-pH)}}, \quad (6)$$

$$u_{eff} = \frac{u_A^0 10^{(pH-pK_{aC})} + u_C^0 10^{(pK_{aA}-pH)}}{1 + 10^{(pH-pK_{aC})} + 10^{(pK_{aA}-pH)}}, \quad (7)$$

for cations, anions and ampholytes, respectively. Where u_c^0 is the ionic mobility of the analyte. The values were not corrected for ionic strength, so they cannot be considered as thermodynamic. The examples of the fitted curves for DBCO-amine and PhOH-N₃ and their reaction product are shown in Figure SI-2. Dissociation parameters of isomeric triazole products of the cycloaddition with AZ-OH were investigated in order to demonstrate the behavior of triazoles. The dissociation constants of the products are very close to those of the reactants. However, the ionic mobility of the triazole product is much lower, due to the increase of hydrodynamic radius. The resulting pK_a values are summarized in Table SI-3.

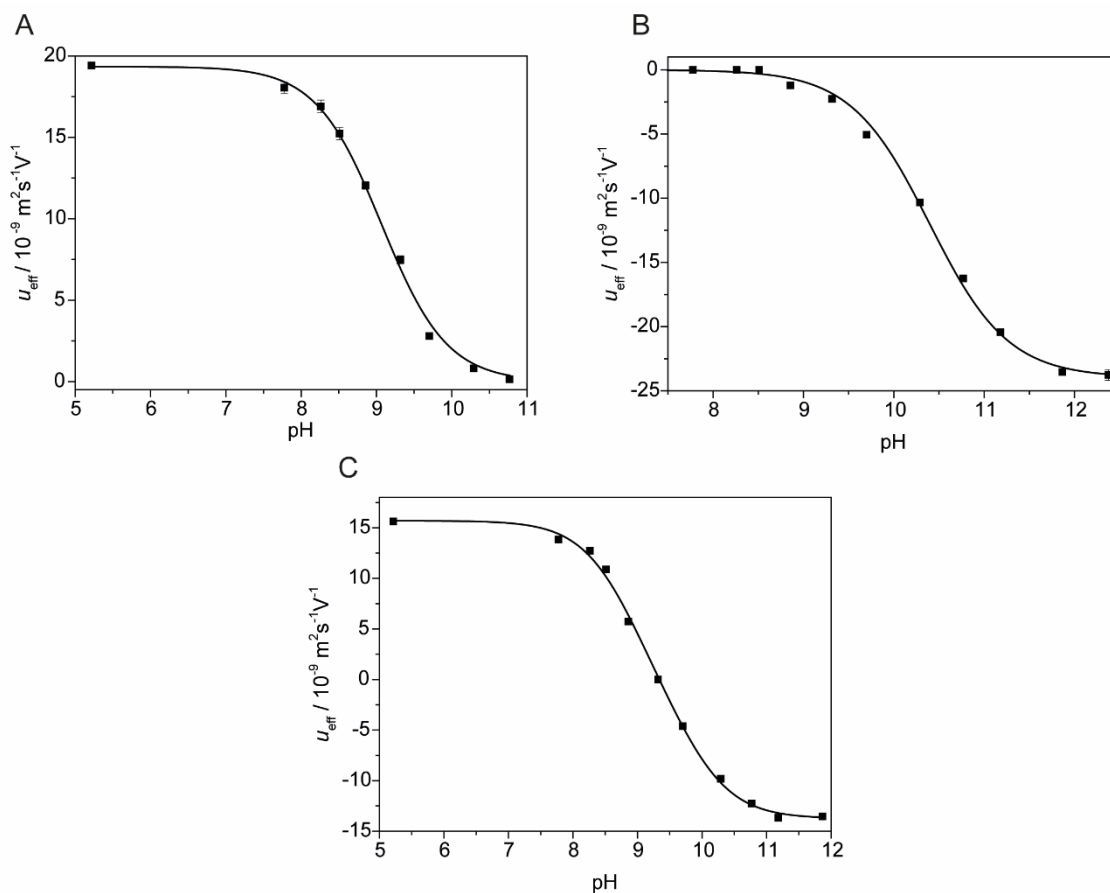


Figure SI-2 The dependence of effective mobility on the pH for A) DBCO-amine, B) PhOH-N₃, C) one of the two regioisomeric triazole reaction products. The solid curves represent fitted dependences according to the equations (5) and (6), respectively.

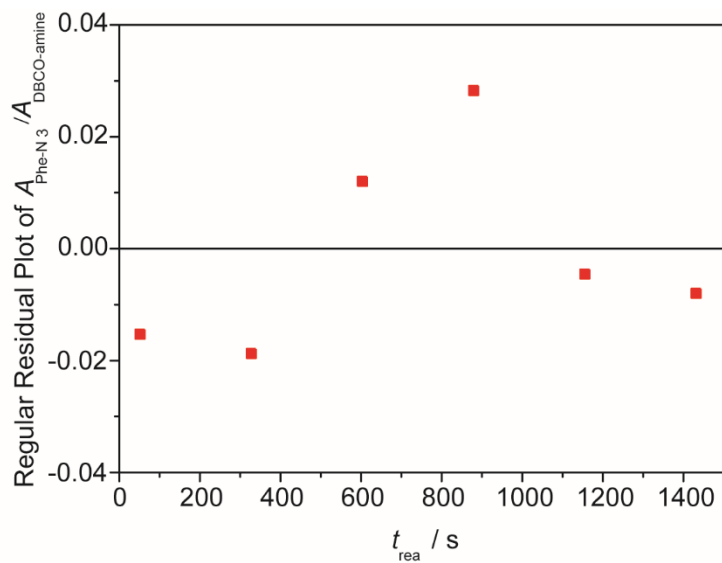


Figure SI-3 Regular residual plot of exponential fit presented in Figure 1, plot of $A_{\text{Phe-N}_3} / A_{\text{DBCO-amine}}$ over time.

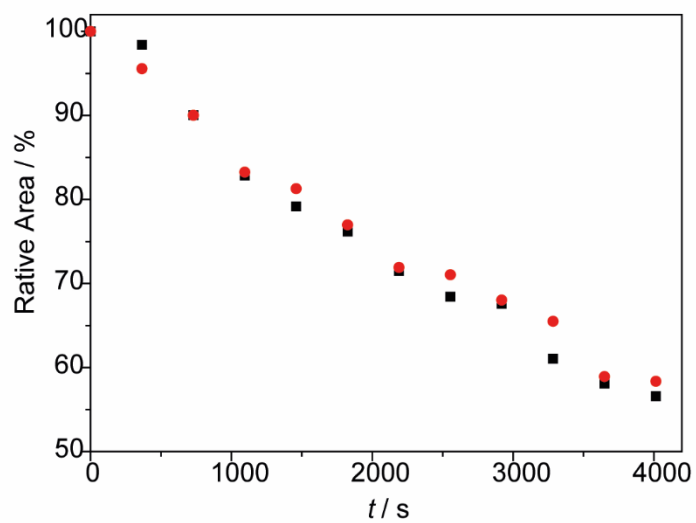


Figure SI-4 Dependence of relative area of AZ peak on time. Black squares: pH 3.77, red circles: pH 11.55.

Table SI-2 Composition, concentrations of the constituents (c), experimental pH and theoretical pH calculated by PeakMaster software of the running buffers for determination of pK_a constants of reactants.

Buffer constituents	Formic a. /LiOH	Formic a. /LiOH	Formic a. /LiOH	Acetic a. /LiOH	Acetic a. /LiOH	Acetic a. /LiOH	Acetic a. /LiOH
<i>c</i> / mM	150 / 7	50 / 9.15	30 / 9.6	60 / 9.9	30 / 10	20 / 10	15 / 10
pH _{exp}	2.87	3.51	3.83	4.51	4.92	5.21	5.51
pH _{theor}	2.56	3.11	3.41	4.01	4.41	4.72	5.02
Buffer constituents	MES /LiOH	MES /LiOH	MOPS /LiOH	Tricine /LiOH	Tricine /LiOH	Tricine /LiOH	
<i>c</i> / mM	45 / 10	20 / 10	20 / 10	40 / 10	20 / 10	15 / 10	
pH _{exp}	5.71	6.25	7.18	7.78	8.26	8.51	
pH _{theor}	5.51	6.05	7.16	7.63	8.11	8.41	
Buffer constituents	CHES /LiOH	CHES /LiOH	β-Alanine /LiOH	β-Alanine /LiOH	β-Alanine /LiOH	LiOH	
<i>c</i> / mM	40 / 10	20 / 10	20 / 10	12 / 10	7 / 10	10	
pH _{exp}	8.86	9.32	10.29	10.77	11.85	12.38	
pH _{theor}	9.03	9.50	10.18	10.75	11.48	11.95	

Table SI-3 pK_a values and ionic mobilities of reactants and products in the SPAAC of PhOH- N_3 and DBCO-amine. The exact composition of the buffers is summarized in Table SI-2. The errors are expressed as standard deviations.

		DBCO-amine	PhOH- N_3	PhCOOH- N_3	Phe- N_3
pK_a	pK_{aC}	9.07 ± 0.03			
	pK_{aA}		10.40 ± 0.03	4.77 ± 0.02	3.54 ± 0.02
u_c^0 $/10^{-9} \text{ m}^2 \text{ s}^{-1} \text{ V}^{-1}$	u_A^0	19.3 ± 0.3			
	u_C^0		-24.0 ± 0.3	22.3 ± 0.2	-21.5 ± 0.2

		Product Triazole 1	Product Triazole 2
pK_a	pK_{aC}	8.82 ± 0.05	$8.69 \pm .07$
	pK_{aA}	9.79 ± 0.06	9.76 ± 0.08
u_c^0 $/10^{-9} \text{ m}^2 \text{ s}^{-1} \text{ V}^{-1}$	u_A^0	13.7 ± 0.4	13.8 ± 0.5
	u_C^0	-15.7 ± 0.5	-15.8 ± 0.6

Table SI-4 Reaction rate constants determined for PhSO₃Na-N₃, PhOH-N₃, PhCOOH-N₃ in dependence on pH and concentration of SDS in MeCN/aqueous buffer. The exact composition of the buffers is summarized in Table SI-1. The errors are expressed as standard deviations.

		PhSO ₃ Na-N ₃		PhOH-N ₃	
pH		3.77	11.58	3.77	11.58
$k /$ (mol dm ⁻³) ⁻¹ s ⁻¹	0 mM SDS	0.322 ± 0.015	0.284 ± 0.004	1.18 ± 0.26	3.96 ± 0.66
	20 mM SDS	0.230 ± 0.004	0.264 ± 0.003	1.93 ± 0.08	3.85 ± 0.26
	50 mM SDS	0.108 ± 0.004	0.170 ± 0.003	2.83 ± 0.12	3.41 ± 0.18

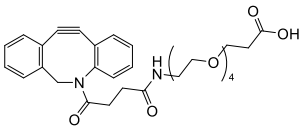
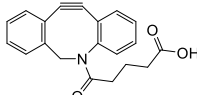
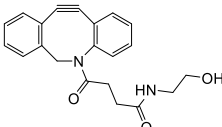
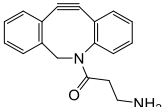
		PhCOOH-N ₃		
pH		3.77	7.09	11.58
$k /$ (mol dm ⁻³) ⁻¹ s ⁻¹	0 mM SDS	0.129 ± 0.008	0.254 ± 0.009	0.190 ± 0.008
	20 mM SDS	0.495 ± 0.010	0.199 ± 0.006	0.173 ± 0.010
	50 mM SDS	0.752 ± 0.040	0.138 ± 0.007	0.168 ± 0.010

Table SI-5 Reaction rate constants determined for Phe-N₃ in dependence on pH and concentration of SDS and NaCl in MeCN/water as well as aqueous buffers. pH is shown for buffers without SDS. For exact composition and parameters of used buffers see Table SI-1. The errors are expressed as standard deviations.

ACN/W	pH	2.29	3.77	7.09	11.55
k (mol dm ⁻³) ⁻¹ s ⁻¹	0 mM SDS	1.35 ± 0.12	1.96 ± 0.09	2.34 ± 0.06	0.865 ± 0.050
	20 mM SDS	2.76 ± 0.08	2.14 ± 0.09	1.85 ± 0.15	0.649 ± 0.082
	50 mM SDS	3.04 ± 0.04	2.12 ± 0.05	0.90 ± 0.12	0.506 ± 0.036
	50mM NaCl	1.27 ± 0.06	1.87 ± 0.03	2.04 ± 0.06	0.885 ± 0.021

WATER	pH	2.39	3.37	6.73	11.49
k (mol dm ⁻³) ⁻¹ s ⁻¹	2 mM SDS	11.4 ± 0.8	4.43 ± 0.28	0.817 ± 0.004	0.466 ± 0.017
	20 mM SDS	10.1 ± 0.9	5.26 ± 0.66	0.345 ± 0.011	0.152 ± 0.010
	50 mM SDS	8.20 ± 0.23	4.91 ± 1.17	0.187 ± 0.009	0.137 ± 0.007

Table SI-6: Comparison of results with rate constants for SPAAC reactions reported in literature.

	alkyne	azide	solvent	additive	rates [M ⁻¹ s ⁻¹]
Heemstra <i>et al.</i> ⁵		PEG ₃ -azide	H ₂ O	none	0.964 – 1.18 ^a
		PEG ₃ -azide	H ₂ O	NaCl (150 mM)	0.967 – 1.38 ^a
		PEG ₃ -azide	H ₂ O	NaCl (500 mM)	1.07 – 1.29 ^a
		PEG ₃ -azide	DMSO (40 %)	none	1.56
		PEG ₃ -azide	DMSO (70 %)	none	1.31
		PEG ₃ -azide	MeCN (40 %)	none	1.10
		PEG ₃ -azide	MeCN (70 %)	none	0.47
van Delft <i>et al.</i> ⁶		benzyl azide	CD ₃ OD	none	0.31
		2-azidopropanoic acid	D ₂ O	NaOD	0.36
van Delft <i>et al.</i> ⁷		benzyl azide	CD ₃ OD	none	0.42
		benzyl azide	D ₂ O:CD ₃ CN 3:1	none	1.9
		benzyl azide	H ₂ O:THF 1:9	none	0.36
		4-azido-N-(2-hydroxyethyl)-3,5-diisopropylbenzamide	CD ₃ OD	none	2.3
		4-azido-N-(2-hydroxyethyl)-3,5-diisopropylbenzamide	D ₂ O:CD ₃ CN 2:1	none	4
this work		4-azidophenol	MeCN/buffer ^b pH = 3.77	none	1.18
		4-azidophenol	MeCN/buffer ^b pH = 11.58	none	3.96
		4-azidophenol	MeCN/buffer ^b pH = 3.77	SDS (50 mM)	2.83
		4-azidophenol	MeCN/buffer ^b pH = 11.58	SDS (50 mM)	3.41
		2-azido-3-phenylpropanoic acid	MeCN/buffer ^b pH = 11.55	SDS (20 mM)	0.649

	2-azido-3-phenylpropanoic acid	H ₂ O/buffer pH = 11.49	SDS (20 mM)	0.152
	2-azido-3-phenylpropanoic acid	MeCN/buffer ^b pH = 2.29	SDS (20 mM)	2.76
	2-azido-3-phenylpropanoic acid	H ₂ O/buffer pH = 2.39	SDS (20 mM)	10.1
	2-azido-3-phenylpropanoic acid	H ₂ O/buffer pH = 2.39	SDS (2 mM)	11.4

^a Rates depend on choice of buffer. ^b Buffers are always aqueous.

4 DFT Calculations

4.1 Ground State Optimization

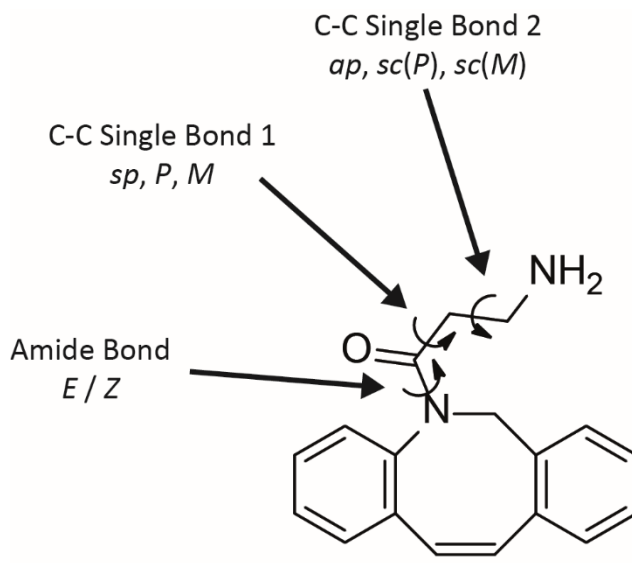


Figure SI-5: Conformational analysis of the cyclooctyne ground state.

4.2 Non-Protonated (NH₂) Cyclooctyne

4.2.1 Amide *E*-Isomer

B3LYP/cc-pVDZ, aug-cc-pVDZ for the oxygen atom, and the NH₂-group, cpcm=acetonitrile

Entry	Conformer	E+ZPE [hartree]	$G_{298\text{ K}}^{\ddagger}$ [hartree]	$\Delta G_{298\text{ K}}^{\ddagger}$ [kJ mol ⁻¹]
1	1 _{sp} -2P _{sc}	-880.037647	-880.083270	6.8
2	1 _{sp} -2M _{sc}	-880.039118	-880.085211	1.7
3	1 _{sp} -2 _{ap}	-880.036603	-880.082568	8.6
4	1P-2P _{sc}	-880.036790	-880.082155	9.7
5	1P-2M _{sc}	-880.036163	-880.081281	12.0
6	1P-2 _{ap}	-880.036668	-880.082489	8.8
7	1M-2P _{sc}	-880.039483	-880.084487	3.6
8	1M-2M _{sc}	-880.039973	-880.085848	0.0
9	1M-2 _{ap}	-880.037473	-880.083131	7.1

4.2.2 Amide Z-Isomer

B3LYP/cc-pVDZ, aug-cc-pVDZ for the oxygen atom, and the NH₂-group, cpcm=acetonitrile

Entry	Conformer	E+ZPE [hartree]	$G_{298\text{ K}}^\ddagger$ [hartree]	$\Delta G_{298\text{ K}}^\ddagger$ [kJ mol ⁻¹]
1	1 _{sp} -2P _{sc}	-880.034827	-880.080275	14.6
2	1 _{sp} -2M _{sc}	-880.034948	-880.080428	14.2
3	1 _{sp} -2 _{ap}	-880.033510	-880.079555	16.5
4	1P-2P _{sc}	-880.035933	-880.080422	14.2
5	1P-2M _{sc}	-880.034025	-880.078876	18.3
6	1P-2 _{ap}	-880.034932	-880.079882	15.7
7	1M-2P _{sc}	-880.032694	-880.077958	20.7
8	1M-2M _{sc}	-880.032417	-880.077736	21.3
9	1M-2 _{ap}	-880.032396	-880.077574	21.7

B3LYP/cc-pVDZ, aug-cc-pVDZ for the oxygen atom, the NH₂-group, and the azide N1 and N3, cpcm=water

Entry	Conformer	E+ZPE [hartree]	$G_{298\text{ K}}^\ddagger$ [hartree]
1	E-1M-2M _{sc}	-880.040232	-880.086010

4.3 Protonated (NH³⁺) Cyclooctyne

B3LYP/cc-pVDZ, aug-cc-pVDZ for the oxygen atom, and the NH₃⁺-group, cpcm=acetonitrile

Entry	Conformer	E+ZPE [hartree]	$G_{298\text{ K}}^\ddagger$ [hartree]	$\Delta G_{298\text{ K}}^\ddagger$ [kJ mol ⁻¹]
1	E-1 _{sp} -2P _{sc}	-880.480420	-880.525848	0.0
2	E-1 _{sp} -2M _{sc}	-880.479465	-880.524263	4.2
3	E-1 _{sp} -2 _{ap}	-880.471742	-880.517054	23.1
4	E-1P-2 _{ap}	-880.469809	-880.515369	27.5
5	E-1M-2P _{sc}	-880.473941	-880.517995	20.6
6	E-1M-2M _{sc}	-880.475267	-880.519650	16.3
7	E-1M-2 _{ap}	-880.470461	-880.515648	27.5
8	Z-1 _{sp} -2P _{sc}	-880.476654	-880.521274	12.0
9	Z-1 _{sp} -2M _{sc}	-880.476059	-880.520786	13.3

B3LYP/cc-pVDZ, aug-cc-pVDZ for the oxygen atom, the NH_3^+ -group, and the azide N1 and N3, cpcm=water

Entry	Conformer	E+ZPE [hartree]	$G_{298\text{ K}}^\ddagger$ [hartree]
1	<i>E</i> -1 _{sp} -2 _{P_{sc}}	-880.481798	-880.527308

4.4 Phenyl Azide

B3LYP/cc-pVDZ, aug-cc-pVDZ for N1 and N3, cpcm=acetonitrile

Entry	E+ZPE [hartree]	$G_{298\text{ K}}^\ddagger$ [hartree]
1	-395.785681	-395.817674

B3LYP/cc-pVDZ, aug-cc-pVDZ for N1 and N3, cpcm=water

Entry	E+ZPE [hartree]	$G_{298\text{ K}}^\ddagger$ [hartree]
1	-395.785748	-395.817741

4.5 Methyl Azide

B3LYP/cc-pVDZ, aug-cc-pVDZ for N1 and N3, cpcm=acetonitrile

Entry	E+ZPE [hartree]	$G_{298\text{ K}}^\ddagger$ [hartree]
1	-204.074819	-204.101374

5 Phenyl Azide (PhN_3) Transition States

5.1 Non-Protonated (NH_2) Cyclooctyne

B3LYP/cc-pVDZ, aug-cc-pVDZ for the oxygen atom, the NH_2 -group, and the azide N1 and N3, cpcm=acetonitrile

Entry	Conformer	E+ZPE [hartree]	$G_{298\text{ K}}^\ddagger$ [hartree]	$\Delta G_{298\text{ K}}^\ddagger$ [kJ mol ⁻¹]	ν_{imag} [cm ⁻¹]
1	<i>E</i> -1 M -2 M_{sc} - <i>anti</i> -11	-1275.815368	-1275.872515	81.4	-313.01
2	<i>E</i> -1 M -2 M_{sc} - <i>syn</i> -11	-1275.814758	-1275.871873	83.1	-323.71

3	<i>E</i> -1 <i>M</i> -2 <i>M</i> _{sc} - <i>syn</i> -12	-1275.816229	-1275.872847	80.5	-337.93
4	<i>Z</i> -1 _{sp} -2 <i>M</i> _{sc} - <i>syn</i> -12	-1275.810180	-1275.868052	93.1	-327.48

B3LYP/cc-pVDZ, aug-cc-pVDZ for the oxygen atom, the NH₂-group, and the azide N1 and N3,
cpcm=water

Entry	Conformer	E+ZPE [hartree]	$G_{298\text{ K}}^\ddagger$ [hartree]	$\Delta G_{298\text{ K}}^\ddagger$ [kJ mol ⁻¹]	ν_{imag} [cm ⁻¹]
1	<i>E</i> -1 <i>M</i> -2 <i>M</i> _{sc} - <i>syn</i> -12	-1275.816553	-1275.873164	80.3	-338.04

5.2 Protonated (NH₃⁺) Cyclooctyne

B3LYP/cc-pVDZ, aug-cc-pVDZ for the oxygen atom, the NH₃⁺-group, and the azide N1 and N3,
cpcm=acetonitrile

Entry	Conformer	E+ZPE [hartree]	$G_{298\text{ K}}^\ddagger$ [hartree]	$\Delta G_{298\text{ K}}^\ddagger$ [kJ mol ⁻¹]	ν_{imag} [cm ⁻¹]
1	<i>E</i> -1 _{sp} -2 <i>P</i> _{sc} - <i>anti</i> -11	-1276.255428	-1276.312442	81.6	-318.02
2	<i>E</i> -1 _{sp} -2 <i>P</i> _{sc} - <i>syn</i> -11	-1276.254292	-1276.311715	83.5	-328.95
3	<i>E</i> -1 _{sp} -2 <i>P</i> _{sc} - <i>syn</i> -12	-1276.255255	-1276.312382	81.8	-332.74
4	<i>Z</i> -1 _{sp} -2 <i>P</i> _{sc} - <i>anti</i> -11	-1276.251469	-1276.308407	92.2	-319.12
5	<i>E</i> -1 _{sp} -2 <i>M</i> _{sc} - <i>syn</i> -11	-1276.255174	-1276.310116	87.7	-359.52

B3LYP/cc-pVDZ, aug-cc-pVDZ for the oxygen atom, the NH₃⁺-group, and the azide N1 and N3,
cpcm=water

Entry	Conformer	E+ZPE [hartree]	$G_{298\text{ K}}^\ddagger$ [hartree]	$\Delta G_{298\text{ K}}^\ddagger$ [kJ mol ⁻¹]	ν_{imag} [cm ⁻¹]
1	<i>E</i> -1 _{sp} -2 <i>P</i> _{sc} - <i>anti</i> -11	-1276.256801	-1276.313665	82.4	-318.11
2	<i>E</i> -1 _{sp} -2 <i>M</i> _{sc} - <i>syn</i> -11	-1276.256381	-1276.311422	88.3	-360.60

6 Methyl Azide (MeN₃) Transition States

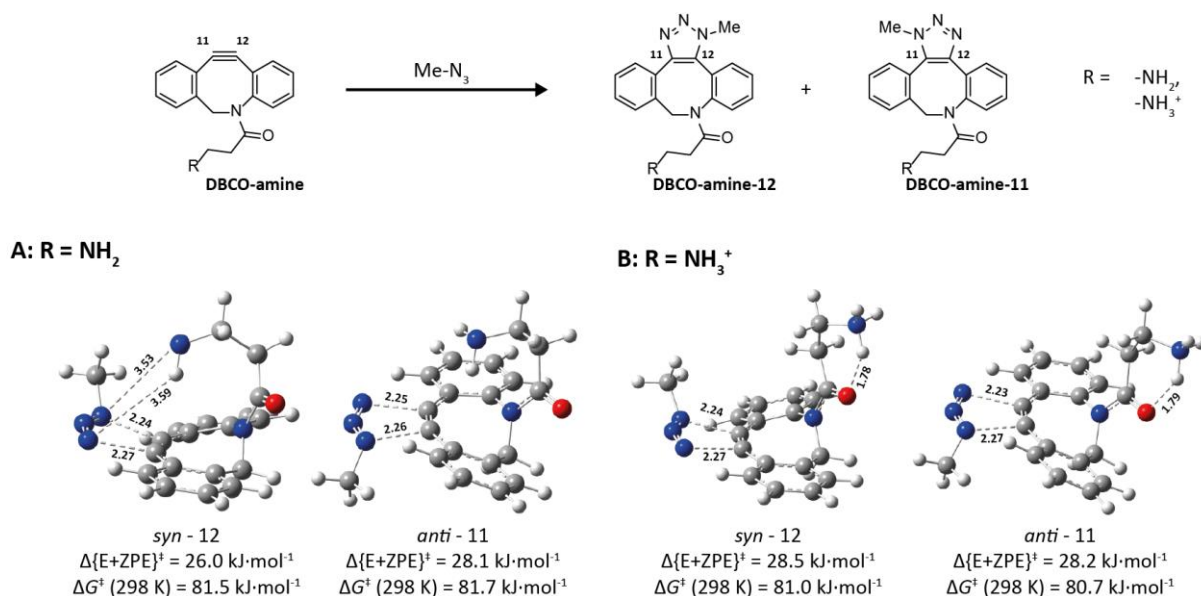


Figure SI-6: Transition state structures of the reaction of methyl azide with non-protonated cyclooctyne (A) and protonated cyclooctyne (B).

6.1 Non-Protonated (NH₂) Cyclooctyne

B3LYP/cc-pVDZ, aug-cc-pVDZ for the oxygen atom, the NH₂-group, and the azide N1 and N3, cpcm=acetonitrile

Entry	Conformer	E+ZPE [hartree]	$G_{298 \text{ K}}^\ddagger$ [hartree]	$\Delta G_{298 \text{ K}}^\ddagger$ [kJ mol ⁻¹]	ν_{imag} [cm ⁻¹]
1	<i>E</i> -1M-2M _{sc} -syn-12	-1084.104878	-1084.156164	81.5	-363.56
2	<i>E</i> -1M-2M _{sc} -anti-11	-1084.104091	-1084.156093	81.7	-355.66

6.2 Protonated (NH₃⁺) cyclooctyne

B3LYP/cc-pVDZ, aug-cc-pVDZ for the oxygen atom, the NH₃⁺-group, and the azide N1 and N3, cpcm=acetonitrile

Entry	Conformer	E+ZPE [hartree]	$G_{298 \text{ K}}^\ddagger$ [hartree]	$\Delta G_{298 \text{ K}}^\ddagger$ [kJ mol ⁻¹]	ν_{imag} [cm ⁻¹]
1	<i>E</i> -1 _{sp} -2P _{sc} -syn-12	-1084.544376	-1084.596376	81.0	-363.48
2	<i>E</i> -1 _{sp} -2P _{sc} -anti-11	-1084.544492	-1084.596481	80.7	-356.75

7 Coordinates of Ground States

7.1 Non-Protonated (NH₂) Cyclooctyne

7.1.1 *E-1_{sp}-2P_{sc}*

C	-2.04624000	-0.45631500	0.68766400
C	-0.71421400	-0.38340900	1.42668500
C	0.22343400	-2.03263200	-0.95588100
C	1.53326500	-1.77854300	-0.45777200
C	1.60622800	-0.66614600	0.43306000
H	-0.42152300	-1.39090700	1.75153900
H	-0.84250700	0.23688100	2.32484900
C	-2.19424700	-1.23276300	-0.49895900
C	-0.97828300	-1.80685800	-0.96737900
C	2.68611200	-2.53964200	-0.70991400
C	2.81092500	-0.38129800	1.07891300
C	3.89108400	-2.21698800	-0.08324700
C	3.95294000	-1.14596600	0.81555300
H	4.89096600	-0.90545300	1.31921600
H	4.78335600	-2.81207100	-0.28666400
H	2.62376700	-3.38785700	-1.39309100
C	-3.44883200	-1.35775700	-1.12002300
H	-3.53765700	-1.95543200	-2.02865500
C	-4.56320800	-0.72025500	-0.57415800
H	-5.53748400	-0.81944900	-1.05681900
C	-4.42785800	0.04843700	0.58786900
H	-5.29766400	0.55160000	1.01533600
C	-3.17849000	0.17854500	1.20516200
H	-3.08006800	0.78521100	2.10827000
C	0.36056200	1.43950900	0.20133100
C	1.46336000	1.94187400	-0.72207200
H	2.41001800	2.00392300	-0.16189500
C	1.14290600	3.30648600	-1.34475800
H	1.88525300	3.50570500	-2.13319100
H	0.15802700	3.26067000	-1.83446700
N	0.44703600	0.14942600	0.66041400
N	1.14029700	4.44564200	-0.41648700
H	0.48373500	4.24779900	0.33688600
H	2.05673900	4.53421200	0.02139200
O	-0.61024200	2.14557300	0.50279900
H	1.62880900	1.18677600	-1.50910400
H	2.85018700	0.45066600	1.78406900

7.1.2 *E-1_{sp}-2M_{sc}*

C	-1.88107900	-0.71393600	0.74326100
C	-0.55397800	-0.63089600	1.48801600
C	0.52840000	-1.73014600	-1.11854500
C	1.80722400	-1.39871400	-0.58664300
C	1.76271000	-0.43457900	0.46460800
H	-0.14039800	-1.64007600	1.61535300
H	-0.73117300	-0.20885100	2.48691900
C	-1.95761800	-1.28720700	-0.56027500
C	-0.69138400	-1.64184000	-1.10761000
C	3.04101600	-1.95184000	-0.96498800

C	2.94161700	-0.07952700	1.12330800
C	4.21372000	-1.56353500	-0.31430900
C	4.16513000	-0.63294200	0.72984000
H	5.08087300	-0.33893200	1.24598400
H	5.16922700	-1.99579200	-0.61722700
H	3.06873000	-2.68807100	-1.76953900
C	-3.19719500	-1.43028900	-1.20659300
H	-3.23218000	-1.87053900	-2.20440000
C	-4.36614400	-1.00914500	-0.57162400
H	-5.32888600	-1.12190600	-1.07406300
C	-4.30110300	-0.43991100	0.70577800
H	-5.21434000	-0.10660100	1.20311100
C	-3.06707100	-0.29294200	1.35000200
H	-3.02324800	0.15767300	2.34401800
C	0.27766100	1.51141800	0.66246800
C	1.26171000	2.32512500	-0.16839500
H	2.04145600	2.72172400	0.50449000
C	0.55971600	3.48425200	-0.88987500
H	0.10623100	4.15660000	-0.14745800
H	1.32259700	4.06465100	-1.43188000
N	0.51560200	0.17119600	0.83009200
N	-0.48635800	3.08580100	-1.84179800
H	-0.10477000	2.43456700	-2.52733300
H	-1.21765000	2.57752500	-1.34607700
O	-0.74141600	2.02982300	1.13555600
H	1.77522000	1.67845500	-0.89566000
H	2.89494000	0.64193800	1.94070400

7.1.3 $E-1_{sp}-2_{ap}$

C	-2.15681000	-0.42267100	0.62709400
C	-0.86376000	-0.56852800	1.42079300
C	0.10277700	-1.85020600	-1.15046400
C	1.39905100	-1.75258100	-0.56889000
C	1.48733500	-0.79954600	0.48992600
H	-0.64193400	-1.63428400	1.56509700
H	-1.00232600	-0.11491200	2.41210500
C	-2.28746600	-0.98357900	-0.67762000
C	-1.08339100	-1.55443300	-1.18029700
C	2.52580500	-2.52093100	-0.90312200
C	2.68078300	-0.67498700	1.20430100
C	3.72091500	-2.35811000	-0.19997200
C	3.79786500	-1.44187200	0.85518900
H	4.72767800	-1.32620300	1.41510100
H	4.59312400	-2.95692000	-0.46883300
H	2.45178500	-3.24691100	-1.71405500
C	-3.51188300	-0.91891100	-1.36416500
H	-3.58892900	-1.35406900	-2.36186400
C	-4.61210900	-0.30060500	-0.76901600
H	-5.56309100	-0.25167400	-1.30314500
C	-4.49226500	0.25970900	0.50812600
H	-5.35069700	0.74832700	0.97375300
C	-3.27276700	0.19947600	1.19260300
H	-3.18480000	0.64432300	2.18629500
C	0.38006900	1.38915900	0.65169500
C	1.55139500	2.00623900	-0.09906400

H	2.38878700	2.13830200	0.60754600
C	1.19672100	3.36136100	-0.72857600
H	0.34942700	3.23094600	-1.42051400
H	0.85853400	4.05364700	0.05555600
N	0.35832600	0.02492200	0.80933300
N	2.29963800	3.99385900	-1.46395600
H	3.09236400	4.14575600	-0.84110000
H	2.63786100	3.36849100	-2.19457700
O	-0.54872400	2.08300600	1.08271800
H	1.91123100	1.31103600	-0.87362000
H	2.73144400	0.03472600	2.03162400

7.1.4 *E-1P-2P_{sc}*

C	2.18249300	-0.05369600	-0.66240100
C	0.82152000	-0.01715000	-1.34752200
C	0.17107700	-2.14334000	0.71854300
C	-1.17859600	-1.95175300	0.30580400
C	-1.40723700	-0.71181400	-0.36168100
H	0.62427700	-0.98691300	-1.82316300
H	0.83874500	0.74920400	-2.13463000
C	2.46597600	-1.00439200	0.36230300
C	1.34205100	-1.79190000	0.74305100
C	-2.23407100	-2.86803200	0.44207100
C	-2.66233200	-0.45112800	-0.91628300
C	-3.49355800	-2.57261300	-0.08293600
C	-3.70656600	-1.37085200	-0.76801200
H	-4.68577000	-1.14802400	-1.19570100
H	-4.30914400	-3.28916900	0.03061100
H	-2.05365100	-3.81290800	0.95659200
C	3.75018600	-1.08452700	0.92713600
H	3.94461300	-1.81869800	1.71064200
C	4.75963400	-0.22814200	0.48609400
H	5.75723300	-0.29217700	0.92511500
C	4.48963400	0.71365100	-0.51360500
H	5.27696600	1.38794500	-0.85688600
C	3.21030100	0.79784200	-1.07548500
H	3.00527100	1.53835600	-1.85171800
C	-0.38474700	1.47318200	0.16239900
C	-1.40482700	1.72148600	1.26379100
H	-2.13042200	0.90409600	1.35819900
C	-2.12744700	3.06871000	1.10187100
H	-2.72788400	3.24917800	2.00703800
H	-1.38015700	3.87390100	1.04271100
N	-0.35058900	0.25309700	-0.46576200
N	-3.01182500	3.17955800	-0.06539300
H	-2.47579600	3.08213300	-0.92656500
H	-3.69355800	2.42233100	-0.06474000
O	0.45243600	2.34173900	-0.11377100
H	-0.81670500	1.74251400	2.19828000
H	-2.81755700	0.48255600	-1.45835400

7.1.5 *E-1P-2M_{sc}*

C	-2.14933100	-0.13447600	0.65090500
C	-0.79343700	-0.08933100	1.34584200

C	-0.10153000	-2.17364600	-0.74645200
C	1.24280000	-1.97441000	-0.32146500
C	1.45322900	-0.74333200	0.36933500
H	-0.58834800	-1.06280500	1.81065400
H	-0.82787800	0.66581000	2.14326100
C	-2.41431500	-1.07388600	-0.38878700
C	-1.27746900	-1.83971200	-0.77530300
C	2.30889200	-2.87638200	-0.46706300
C	2.70182500	-0.47887100	0.93586600
C	3.56189800	-2.57608700	0.07083900
C	3.75716900	-1.38437400	0.77769400
H	4.73145600	-1.15812200	1.21465000
H	4.38612200	-3.28146600	-0.05015900
H	2.14205500	-3.81412400	-0.99893800
C	-3.69497800	-1.16504100	-0.96025400
H	-3.87503600	-1.89055400	-1.75518700
C	-4.71911900	-0.33089700	-0.51082600
H	-5.71398300	-0.40370300	-0.95465900
C	-4.46737500	0.59992200	0.50396200
H	-5.26629300	1.25680900	0.85419900
C	-3.19180000	0.69511400	1.07224500
H	-3.00115100	1.42697400	1.86031200
C	0.41319300	1.43580400	-0.13131800
C	1.50062000	1.73927900	-1.14445600
H	2.02895200	0.83069200	-1.46221800
C	2.52517800	2.77913200	-0.62692700
H	3.00434800	2.39640900	0.28771700
H	3.32149100	2.86994700	-1.38197600
N	0.38472300	0.20729900	0.48158900
N	2.00218000	4.11952600	-0.34593800
H	1.64034200	4.52864400	-1.20697600
H	1.19400700	4.04286800	0.27100300
O	-0.45608800	2.28103900	0.12755400
H	0.98793500	2.15964400	-2.02412900
H	2.84366100	0.44406500	1.49943100

7.1.6 *E-1P-2_{ap}*

C	-2.27835500	-0.02284000	0.62095200
C	-0.95961800	-0.11207700	1.37987000
C	-0.26796700	-2.04971100	-0.84839000
C	1.06355600	-1.95371500	-0.35271100
C	1.29925100	-0.79649300	0.44851000
H	-0.82748500	-1.13160000	1.76557100
H	-0.99563600	0.57254900	2.23852900
C	-2.53689800	-0.85667300	-0.50684600
C	-1.42232800	-1.64998000	-0.90286200
C	2.09481900	-2.88864300	-0.53593200
C	2.53472900	-0.63735000	1.07961800
C	3.33735300	-2.69245400	0.07023600
C	3.55597100	-1.57394900	0.88227400
H	4.52105100	-1.43043200	1.37158800
H	4.13468300	-3.42248000	-0.08101800
H	1.90977900	-3.76920200	-1.15275400
C	-3.78849000	-0.82754800	-1.14518000
H	-3.96414900	-1.47343200	-2.00696700

C	-4.78955600	0.02395600	-0.67649100
H	-5.76170200	0.04523900	-1.17300300
C	-4.54320200	0.85224300	0.42464300
H	-5.32367900	1.52289600	0.79002400
C	-3.29621000	0.82757200	1.06019300
H	-3.10885900	1.48086800	1.91524300
C	0.39974000	1.47019000	0.11018800
C	1.54012400	1.79331400	-0.83909600
H	2.04658500	0.89048700	-1.20596300
C	2.56988500	2.75397800	-0.20862000
H	2.04637300	3.65206700	0.15332400
H	3.03095000	2.27657500	0.67024500
N	0.27231600	0.19355600	0.59837000
N	3.64610100	3.17302100	-1.11078300
H	4.15100200	2.35733200	-1.45532300
H	3.25581400	3.62930200	-1.93447600
O	-0.42350300	2.34374500	0.41364800
H	1.07395100	2.29558700	-1.70217800
H	2.69360100	0.22932700	1.72272500

7.1.7 *E-1M-2P_{sc}*

C	1.91095900	-0.48438100	-0.83276800
C	0.59195100	-0.33582400	-1.58098000
C	-0.51598500	-1.69399300	0.87522800
C	-1.78750100	-1.30520600	0.36494800
C	-1.73090700	-0.22626900	-0.56852100
H	0.17685000	-1.32824200	-1.80037700
H	0.77716700	0.17365900	-2.53632700
C	1.97460800	-1.18350600	0.40916300
C	0.70376400	-1.60488500	0.89675000
C	-3.02438000	-1.89665200	0.66659300
C	-2.90357000	0.19639300	-1.19848700
C	-4.19083000	-1.43641500	0.05324400
C	-4.13090300	-0.39590200	-0.88060600
H	-5.04071200	-0.04656100	-1.37209200
H	-5.14934000	-1.89838200	0.29665700
H	-3.05888000	-2.71853000	1.38302900
C	3.20485900	-1.37132400	1.06191800
H	3.23021900	-1.90896600	2.01109200
C	4.37710400	-0.87118200	0.49355100
H	5.33253900	-1.01768900	1.00106800
C	4.32479600	-0.18048800	-0.72294700
H	5.24079100	0.21469500	-1.16693100
C	3.10004200	0.01146200	-1.37290600
H	3.06497000	0.55917600	-2.31712400
C	-0.23287500	1.73767800	-0.59193800
C	-1.14014200	2.46942800	0.38288100
H	-0.82880900	3.52303400	0.35274400
C	-1.00258800	1.92124400	1.82464400
H	-1.56287500	2.59598800	2.49107300
H	-1.48463400	0.93602000	1.89676300
N	-0.47831500	0.40960100	-0.85726600
N	0.36618100	1.78792700	2.33472600
H	0.87196100	1.07865300	1.80619200
H	0.88032400	2.65849100	2.20687400

O	0.77628700	2.28445300	-1.05228300
H	-2.19542900	2.41888400	0.07932400
H	-2.84993800	1.00038900	-1.93452700

7.1.8 $E-1M-2M_{sc}$

C	1.96455300	-0.44682200	-0.79647600
C	0.65353100	-0.30824100	-1.55954300
C	-0.46021300	-1.73443900	0.84983000
C	-1.73285300	-1.35692800	0.33380100
C	-1.68740600	-0.26958600	-0.58912900
H	0.26260800	-1.30441500	-1.80395500
H	0.84298500	0.22302000	-2.50195800
C	2.02813700	-1.18208500	0.42400000
C	0.75854200	-1.63487000	0.88593000
C	-2.96102800	-1.97892300	0.61148900
C	-2.85865800	0.12558200	-1.24046400
C	-4.12771400	-1.54362500	-0.01898700
C	-4.07614500	-0.49831000	-0.94846600
H	-4.98521700	-0.16865400	-1.45469800
H	-5.07874600	-2.03003200	0.20530700
H	-2.98718100	-2.80786400	1.32012800
C	3.25514200	-1.37294700	1.08145900
H	3.28024000	-1.93960600	2.01364100
C	4.42458900	-0.83835900	0.53944200
H	5.37785900	-0.98718500	1.05036800
C	4.37220800	-0.10948800	-0.65457800
H	5.28597300	0.31308700	-1.07746400
C	3.15055500	0.08428700	-1.30967000
H	3.11551900	0.65975800	-2.23718700
C	-0.24909600	1.74302900	-0.59657100
C	-1.20793000	2.49109500	0.31175000
H	-1.33384900	3.49663100	-0.11665100
C	-0.60200600	2.61678900	1.73042100
H	0.40110000	3.06524600	1.65455400
H	-1.22694400	3.31810700	2.30493400
N	-0.44728800	0.40438900	-0.84588200
N	-0.49607600	1.36659400	2.48963400
H	-1.41498100	0.93477800	2.57949700
H	0.07431400	0.68788800	1.98768500
O	0.76642800	2.30837600	-1.02150500
H	-2.19517100	2.01940600	0.38269500
H	-2.81164200	0.93900000	-1.96654400

7.1.9 $E-1M-2_{ap}$

C	2.12599300	-0.53143500	-0.60993900
C	0.85434200	-0.68518000	-1.43613100
C	-0.31265400	-1.49030000	1.24445900
C	-1.57227500	-1.37246700	0.59048600
C	-1.53674300	-0.58112900	-0.59649100
H	0.54140500	-1.73772200	-1.43493800
H	1.06816300	-0.39714500	-2.47474500
C	2.15926600	-0.89879500	0.76764100
C	0.89250800	-1.28766200	1.28951200

C	-2.77298600	-1.99202000	0.97369000
C	-2.68441400	-0.47776000	-1.38642100
C	-3.92016600	-1.84436500	0.19244700
C	-3.87516000	-1.09580000	-0.98972000
H	-4.76732000	-0.99579500	-1.61054200
H	-4.85014000	-2.32667700	0.49913400
H	-2.79283100	-2.59305400	1.88384500
C	3.35837500	-0.83130800	1.49711700
H	3.35985900	-1.11631000	2.55042600
C	4.52977500	-0.40141900	0.87288400
H	5.46111400	-0.35025200	1.44033400
C	4.50659800	-0.03222500	-0.47713200
H	5.42125400	0.30881100	-0.96655200
C	3.31244700	-0.09461800	-1.20470200
H	3.30087200	0.20135800	-2.25602200
C	-0.21965900	1.46544800	-1.00153000
C	-1.28033300	2.28968200	-0.29502600
H	-1.20950300	3.31372300	-0.68796800
C	-1.02191600	2.29771800	1.23089100
H	-1.03935900	1.26424700	1.60881600
H	-0.00949400	2.68863200	1.42100100
N	-0.32917900	0.09528100	-0.97507600
N	-1.97800000	3.08897200	2.00869600
H	-1.98575500	4.05378800	1.68028700
H	-2.92301700	2.73550900	1.86416700
O	0.78156900	2.00292900	-1.49171000
H	-2.29516700	1.91578100	-0.48215400
H	-2.64038000	0.10370500	-2.30897300

7.1.10 $Z-1_{sp}-2P_{sc}$

C	-1.64367300	-0.90506500	0.72627100
C	-0.35260900	-0.42669500	1.38842700
C	0.90474400	-1.88530400	-0.94666500
C	2.12035600	-1.29377200	-0.49790000
C	1.93334200	-0.15357200	0.33389500
H	0.21200400	-1.30427300	1.73044000
H	-0.60832600	0.15276400	2.28740700
C	-1.62168800	-1.73344100	-0.43423900
C	-0.31363400	-1.98208000	-0.93979700
C	3.41938500	-1.77052600	-0.74200900
C	3.04261100	0.46262000	0.91470100
C	4.51891300	-1.13028900	-0.16983800
C	4.33102200	-0.01898800	0.66142900
H	5.19071600	0.47545800	1.11773800
H	5.52592700	-1.50423200	-0.36418800
H	3.55270700	-2.64829600	-1.37597900
C	-2.81831800	-2.22061000	-0.98440500
H	-2.77886900	-2.85121500	-1.87397100
C	-4.04122000	-1.90067500	-0.39170100
H	-4.96954100	-2.28214800	-0.82132100
C	-4.07408400	-1.09383600	0.75028900
H	-5.02837100	-0.84342000	1.21784600
C	-2.88285200	-0.60204700	1.29838600
H	-2.91966000	0.03142800	2.18811900
C	0.32237800	1.62193100	0.08391500

C	-1.01202400	2.23769000	0.47633100
H	-1.82965600	1.56495200	0.17631100
C	-1.23360900	3.62402000	-0.13918900
H	-2.13778900	4.05921300	0.31399300
H	-0.39140700	4.28072100	0.12522400
N	0.60955300	0.36505000	0.56673100
N	-1.39247300	3.64809700	-1.59966800
H	-0.56874200	3.22511700	-2.02438100
H	-2.18335400	3.06446400	-1.87046700
O	1.12362100	2.23534300	-0.63243500
H	-1.05741100	2.29826700	1.57813100
H	2.88900800	1.33027300	1.55774900

7.1.11 $Z-1_{sp}-2M_{sc}$

C	-1.80147900	-0.70294500	0.68130000
C	-0.48477000	-0.24844100	1.30616800
C	0.67918000	-2.15942100	-0.72495200
C	1.93441700	-1.60567400	-0.34083900
C	1.83372300	-0.33483800	0.29336300
H	-0.00748400	-1.11148400	1.78912100
H	-0.69847600	0.47873600	2.10311100
C	-1.83285500	-1.70802600	-0.33018600
C	-0.54304400	-2.15029100	-0.74243200
C	3.19163900	-2.21972300	-0.46935500
C	2.98222800	0.27540900	0.79845100
C	4.33311000	-1.58699200	0.02410300
C	4.22868600	-0.34445200	0.66145600
H	5.12088000	0.14543200	1.05611400
H	5.30746000	-2.06817600	-0.07991800
H	3.25951100	-3.19604800	-0.95137900
C	-3.05812600	-2.16515000	-0.84141100
H	-3.05996300	-2.93315000	-1.61646700
C	-4.25719400	-1.63942800	-0.35645700
H	-5.20808100	-1.99769000	-0.75566900
C	-4.23763200	-0.65569000	0.63753400
H	-5.17353200	-0.24296300	1.01933000
C	-3.01716300	-0.19398000	1.14609900
H	-3.01251700	0.57732500	1.92022200
C	0.36778100	1.47281200	-0.32748600
C	-0.93150100	2.23803700	-0.12347200
H	-1.75234400	1.64718400	-0.56231200
C	-0.89668500	3.63395600	-0.75680800
H	-0.68321000	3.53834500	-1.83147100
H	-1.90044300	4.07701800	-0.66397000
N	0.55612800	0.32169700	0.40178400
N	0.07734000	4.56889100	-0.17848600
H	-0.10054800	4.68227200	0.81892700
H	1.00943000	4.16530600	-0.25789400
O	1.22340600	1.87611400	-1.12548500
H	-1.15685700	2.31874700	0.95254000
H	2.89277400	1.24513900	1.29004100

7.1.12 Z-1_{sp}-2_{ap}

C	-1.46928400	-1.04498700	0.69418800
C	-0.26840000	-0.33982100	1.31965600
C	1.24412700	-1.91855300	-0.75845700
C	2.35921700	-1.11986000	-0.37318500
C	2.00169000	0.09051900	0.28663900
H	0.38576900	-1.09548700	1.77432200
H	-0.61893600	0.30477100	2.13915400
C	-1.30202900	-2.01270400	-0.33999300
C	0.04759000	-2.16836900	-0.76851600
C	3.71564500	-1.45319000	-0.52595600
C	3.00383800	0.92091200	0.79001900
C	4.70535100	-0.60207900	-0.03343900
C	4.35062500	0.58054900	0.62746800
H	5.12513600	1.24136900	1.02147600
H	5.75756600	-0.86540300	-0.15672300
H	3.98057500	-2.38525100	-1.02722200
C	-2.41090300	-2.70334600	-0.85494700
H	-2.26123200	-3.43820300	-1.64748300
C	-3.68790700	-2.44849000	-0.35137500
H	-4.54796800	-2.98739000	-0.75357600
C	-3.86249400	-1.50474100	0.66623600
H	-4.85953500	-1.30464300	1.06360500
C	-2.75912100	-0.81097400	1.17880100
H	-2.90667600	-0.07323100	1.97129100
C	0.18125700	1.57655400	-0.25728500
C	-1.24451100	2.03918500	-0.00823700
H	-1.93428200	1.28570800	-0.42235100
C	-1.54877800	3.40992700	-0.62485300
H	-0.85681700	4.16057300	-0.21314800
H	-1.36266600	3.37350600	-1.70795100
N	0.61654000	0.46008200	0.42326400
N	-2.92470400	3.87689700	-0.40515100
H	-3.58685900	3.20347300	-0.78915500
H	-3.12417500	3.92160100	0.59361800
O	0.91964000	2.18116500	-1.04371600
H	-1.44465100	2.06526300	1.07597500
H	2.71929400	1.84198500	1.30051700

7.1.13 Z-1P-2P_{sc}

C	-1.53521600	-0.68223300	0.87600300
C	-0.21785500	-0.19867700	1.47715300
C	0.94118300	-1.72953200	-0.87007400
C	2.17851600	-1.14533600	-0.47246500
C	2.02786600	0.01609900	0.33595900
H	0.35566200	-1.07048300	1.81888800
H	-0.42724300	0.40788800	2.36986200
C	-1.56294800	-1.52938600	-0.27123400
C	-0.27726800	-1.81035900	-0.81592800
C	3.46433100	-1.64436600	-0.73840500
C	3.15680300	0.63240800	0.87485900
C	4.58538300	-1.00504000	-0.20750500
C	4.43250800	0.12732900	0.60194500
H	5.30960000	0.62080100	1.02489900
H	5.58255000	-1.39631900	-0.41767000

H	3.57147800	-2.53808700	-1.35473600
C	-2.78519400	-1.98670700	-0.78951400
H	-2.78412900	-2.62655900	-1.67311800
C	-3.98543100	-1.62190400	-0.17592600
H	-4.93378800	-1.97792500	-0.58255200
C	-3.96914900	-0.80584300	0.96011000
H	-4.90464000	-0.52584700	1.44802200
C	-2.75149200	-0.34402600	1.47655500
H	-2.75237300	0.29424000	2.36354100
C	0.41637300	1.76804900	0.00772000
C	-0.88310600	2.47610500	0.35581100
H	-1.48884600	1.94842000	1.09874200
C	-1.72389400	2.76516600	-0.90498300
H	-2.58166000	3.38893800	-0.60897800
H	-1.11729800	3.35830300	-1.60546800
N	0.71475700	0.55729200	0.58671800
N	-2.23474100	1.58962000	-1.61977900
H	-1.46306100	1.00154800	-1.93169000
H	-2.78810800	1.00829400	-0.99249100
O	1.19314200	2.30407200	-0.79374300
H	-0.58083500	3.43723200	0.80479800
H	3.02898500	1.51812600	1.49883100

7.1.14 Z-1P-2M_{sc}

C	-1.55596400	-0.84456100	0.81385800
C	-0.24253800	-0.43098800	1.47174200
C	0.93504000	-1.66541900	-1.02991600
C	2.16514700	-1.11498100	-0.56607300
C	2.00192800	-0.05563200	0.37095000
H	0.33722800	-1.33387600	1.70535000
H	-0.45787400	0.06087700	2.43165900
C	-1.57396200	-1.55213700	-0.42454900
C	-0.28313200	-1.75959600	-0.99024800
C	3.45663600	-1.56315100	-0.88925800
C	3.12488600	0.50931900	0.97493100
C	4.57115600	-0.97364600	-0.29118100
C	4.40631600	0.05646200	0.64293200
H	5.27846700	0.51019100	1.11749000
H	5.57265000	-1.32470300	-0.54704400
H	3.57341100	-2.37894700	-1.60410700
C	-2.79139500	-1.95536500	-0.99596400
H	-2.78349200	-2.48937600	-1.94735500
C	-3.99532200	-1.67253000	-0.34765800
H	-4.94018900	-1.98571000	-0.79587100
C	-3.98780100	-0.99116700	0.87349000
H	-4.92687600	-0.77246400	1.38551200
C	-2.77547900	-0.58285800	1.44348400
H	-2.78277900	-0.04792800	2.39636400
C	0.36131100	1.69786100	0.24060000
C	-0.98254200	2.29595600	0.60480500
H	-1.43564700	1.82659900	1.48591600
C	-1.98081300	2.23518700	-0.58264700
H	-2.11843000	1.18829800	-0.89012300
H	-2.95730700	2.58666600	-0.21528200

N	0.68314200	0.43537800	0.68274500
N	-1.62048800	3.02098800	-1.76541000
H	-1.54937700	4.00585700	-1.51132500
H	-0.68488400	2.75873500	-2.07424200
O	1.14011100	2.34221600	-0.47773900
H	-0.79273700	3.35193200	0.85034500
H	2.98752500	1.31502000	1.69749600

7.1.15 Z-1P-2_{ap}

C	-1.41350400	-0.78330600	0.83159600
C	-0.13635200	-0.20139900	1.43019900
C	1.15590200	-1.74267700	-0.82295400
C	2.34315600	-1.04998200	-0.44659700
C	2.10232400	0.13609900	0.30335000
H	0.48872900	-1.02409700	1.80185000
H	-0.39312600	0.41659900	2.30269700
C	-1.36762300	-1.67953700	-0.27710100
C	-0.05519700	-1.90355900	-0.78354000
C	3.66414800	-1.46410200	-0.68494500
C	3.18008800	0.86149600	0.81060000
C	4.73200000	-0.71656700	-0.18677200
C	4.49127700	0.44083000	0.56370800
H	5.32712700	1.01974900	0.96112200
H	5.75656300	-1.04217000	-0.37632200
H	3.84069800	-2.37696000	-1.25560000
C	-2.55034700	-2.22994100	-0.79667300
H	-2.49387000	-2.90750700	-1.64990800
C	-3.78219500	-1.90674600	-0.22439500
H	-4.69991600	-2.33428400	-0.63262100
C	-3.83734600	-1.04003200	0.87217900
H	-4.79783500	-0.79154200	1.32788700
C	-2.65946700	-0.48731100	1.39120200
H	-2.71609600	0.18835200	2.24829000
C	0.35928100	1.74524600	-0.10863600
C	-1.03215400	2.29155200	0.14620500
H	-1.47651900	1.92616400	1.07921100
C	-1.97886200	1.97803900	-1.03811600
H	-1.58092900	2.46132200	-1.94365900
H	-1.98610000	0.89501100	-1.22934100
N	0.75178700	0.58808000	0.52412800
N	-3.36416700	2.40913000	-0.84114800
H	-3.76835300	1.91783700	-0.04485800
H	-3.39758500	3.40155000	-0.61140500
O	1.10411500	2.32911900	-0.90743200
H	-0.92326300	3.38317900	0.23558300
H	2.98344800	1.76476100	1.38979800

7.1.16 Z-1M-2P_{sc}

C	1.91322400	-0.40903600	-0.59291100
C	0.56375000	0.04956400	-1.14274100
C	-0.43213100	-2.30190800	0.49486900
C	-1.73008500	-1.80370800	0.18469300
C	-1.74069300	-0.43671400	-0.21177300

H	0.16385300	-0.73747200	-1.79609300
H	0.72082900	0.93164700	-1.77973300
C	2.03020500	-1.57043600	0.22648600
C	0.78391700	-2.18647000	0.53514800
C	-2.92610400	-2.54086800	0.16932500
C	-2.93521400	0.14771700	-0.63407600
C	-4.11589700	-1.93548600	-0.23648000
C	-4.11999000	-0.59547500	-0.64317300
H	-5.04894800	-0.12524100	-0.97128800
H	-5.04240500	-2.51270200	-0.24532100
H	-2.90815900	-3.58929100	0.47042500
C	3.29055800	-2.01221700	0.66025100
H	3.35654300	-2.90117900	1.28946100
C	4.44249600	-1.31928100	0.28320100
H	5.42053700	-1.66605000	0.62238600
C	4.34090600	-0.18545000	-0.52879200
H	5.23953400	0.35635300	-0.83012600
C	3.08492000	0.26105100	-0.95876600
H	3.01786200	1.14651600	-1.59615100
C	-0.46907000	1.36317000	0.75547000
C	0.65463200	2.37347900	0.65292000
H	0.80179900	2.79167700	1.65868400
C	0.27167000	3.51714500	-0.32216900
H	1.14835100	4.17377400	-0.43253200
H	0.06428300	3.09761800	-1.31984800
N	-0.52994500	0.34398700	-0.16908100
N	-0.87369200	4.34060200	0.07388900
H	-1.69008400	3.75142000	0.23399700
H	-0.68174400	4.78390500	0.97159400
O	-1.35633800	1.51220000	1.60665300
H	1.60285600	1.92560100	0.33451800
H	-2.93150100	1.19323000	-0.94574500

7.1.17 Z-1M-2M_{sc}

C	1.83135900	-0.48176600	-0.58232900
C	0.51987800	0.11197400	-1.09282000
C	-0.65245700	-2.25074100	0.39615000
C	-1.90834200	-1.63502400	0.12727200
C	-1.81561100	-0.24827300	-0.17991400
H	0.05698500	-0.60330900	-1.78573900
H	0.73966300	1.01535900	-1.67889300
C	1.85913400	-1.69939800	0.15949400
C	0.56887800	-2.23456700	0.43624800
C	-3.15738300	-2.27612600	0.07496300
C	-2.96418700	0.45241000	-0.54851900
C	-4.29924100	-1.55657600	-0.27868900
C	-4.20276900	-0.19599400	-0.59484800
H	-5.09455700	0.36548700	-0.87955800
H	-5.26721500	-2.05983700	-0.31611500
H	-3.21860400	-3.34026000	0.30726000
C	3.08183300	-2.26622800	0.55374000
H	3.07922200	-3.19688400	1.12326200
C	4.28350500	-1.64250700	0.21324200
H	5.23231200	-2.08629400	0.52088000
C	4.26888000	-0.45301500	-0.52200000

H	5.20650800	0.03527200	-0.79459200
C	3.05087700	0.11759200	-0.91237400
H	3.05240500	1.04488100	-1.49103400
C	-0.40019400	1.35519000	0.91692900
C	0.82469400	2.25127500	0.95021700
H	1.13827000	2.30132700	2.00392600
C	0.46827800	3.67798300	0.47102800
H	-0.38392300	4.04996200	1.06086200
H	1.32443100	4.33408300	0.69141700
N	-0.54656200	0.43328300	-0.09486000
N	0.14274000	3.81927700	-0.95212500
H	0.92596000	3.51743500	-1.52893700
H	-0.64836000	3.23037600	-1.20646400
O	-1.28066100	1.51045100	1.77346000
H	1.67167700	1.86899800	0.37210600
H	-2.88551800	1.51462600	-0.78390000

7.1.18 Z-1M-2_{ap}

C	1.62833900	-0.80266400	-0.57541100
C	0.42995700	-0.01548600	-1.10231500
C	-1.10756400	-2.12899000	0.43476300
C	-2.24823600	-1.32646800	0.14455200
C	-1.93315700	0.01962200	-0.19359100
H	-0.13849100	-0.65884900	-1.78715700
H	0.79674900	0.82927300	-1.70229300
C	1.46037900	-1.99140100	0.19384000
C	0.10094600	-2.30600700	0.47853300
C	-3.58388800	-1.76010900	0.09644900
C	-2.95199600	0.88661400	-0.58985400
C	-4.59344600	-0.87521100	-0.28358300
C	-4.27814100	0.44422500	-0.63135600
H	-5.06728600	1.13325000	-0.93834400
H	-5.62954900	-1.21725000	-0.31799400
H	-3.81621600	-2.79499600	0.35184400
C	2.57687100	-2.73777700	0.60400500
H	2.42588300	-3.64280000	1.19443800
C	3.86279100	-2.32319600	0.25223100
H	4.72817200	-2.90668000	0.57238000
C	4.03904500	-1.16436400	-0.51042100
H	5.04266100	-0.83968100	-0.79203400
C	2.92792200	-0.41445200	-0.91652500
H	3.07666300	0.48820200	-1.51519500
C	-0.28432300	1.43278300	0.84424800
C	1.06129000	2.12986200	0.79527900
H	1.27261400	2.47919500	1.81579100
C	1.01535100	3.34720800	-0.15894100
H	0.74969800	3.01548400	-1.17546500
H	0.21430100	4.02828300	0.16902200
N	-0.57292900	0.49032200	-0.11757900
N	2.26557600	4.10566300	-0.23945600
H	2.53066400	4.44322700	0.68499400
H	3.02478400	3.49803900	-0.54482200
O	-1.12118500	1.76433500	1.69395800
H	1.87533700	1.45950300	0.49513100
H	-2.69787600	1.91410000	-0.85413600

7.1.19 E-1M-2Msc (water)

C	1.96553200	-0.44675300	-0.79577200
C	0.65457100	-0.30893600	-1.55910700
C	-0.45939000	-1.73243600	0.85198400
C	-1.73207400	-1.35652200	0.33480300
C	-1.68671200	-0.27046100	-0.58958100
H	0.26388400	-1.30534500	-1.80286000
H	0.84397200	0.22151600	-2.50197400
C	2.02894900	-1.18005200	0.42592700
C	0.75933300	-1.63235200	0.88838400
C	-2.95997700	-1.97901200	0.61252800
C	-2.85762400	0.12290800	-1.24254700
C	-4.12645000	-1.54545300	-0.01955500
C	-4.07486300	-0.50150800	-0.95059000
H	-4.98375100	-0.17326800	-1.45804600
H	-5.07730800	-2.03220500	0.20467600
H	-2.98613500	-2.80697900	1.32229800
C	3.25593900	-1.37014600	1.08369000
H	3.28095500	-1.93534000	2.01676700
C	4.42559600	-0.83694600	0.54069300
H	5.37883600	-0.98530200	1.05180400
C	4.37347900	-0.11036100	-0.65475000
H	5.28744000	0.31079700	-1.07862000
C	3.15182000	0.08271600	-1.31010800
H	3.11713400	0.65602100	-2.23900000
C	-0.24928800	1.74255600	-0.59736700
C	-1.20948600	2.49107800	0.30916600
H	-1.33486800	3.49632500	-0.12003600
C	-0.60586200	2.61781900	1.72867900
H	0.39799700	3.06487100	1.65418600
H	-1.23092800	3.32060600	2.30119600
N	-0.44665400	0.40393900	-0.84618000
N	-0.50309500	1.36825400	2.48961300
H	-1.42312200	0.93864000	2.57880500
H	0.06597100	0.68776200	1.98853100
O	0.76683800	2.30811700	-1.02121800
H	-2.19680800	2.01949800	0.37892400
H	-2.81067900	0.93526400	-1.96980400

7.2 Protonated (NH₃⁺) Cyclooctyne

7.2.1 E-1_{sp}-2P_{sc}

C	-0.62248700	-0.52816500	1.43983400
C	1.71649300	-0.55214000	0.42581300
C	1.73213100	-1.64315300	-0.49216400
C	-1.94495300	-0.67839300	0.69909100
C	-2.03040300	-1.42822400	-0.51059100
H	-0.23569600	-1.51746400	1.71567400
H	-0.78916200	0.04188400	2.36379400
C	-0.77112000	-1.88560000	-0.99291300
C	0.44613800	-2.00059400	-0.98784500
C	-4.35503900	-0.34655900	0.60366600
H	-5.26069800	0.07884900	1.04070200
C	-4.42998800	-1.09100600	-0.57930700

H	-5.39325600	-1.24850400	-1.06834400
C	4.12518900	-1.86321000	-0.15123300
C	4.09927900	-0.81064000	0.77025700
H	5.01730400	-0.49271700	1.26730600
C	-3.12039800	-0.14182700	1.23049000
C	-3.27081500	-1.62924000	-1.13914600
C	2.89406700	-0.16321200	1.06531700
C	2.94845100	-2.28531300	-0.77313600
H	-3.06847500	0.44505600	2.15022400
H	-3.31389100	-2.20500400	-2.06492000
H	2.86447100	0.65154700	1.79069000
H	2.95854000	-3.11919100	-1.47614300
H	5.06665000	-2.36677000	-0.37802500
N	0.48350200	0.14143600	0.68741100
C	0.29574300	1.43472600	0.32954800
C	1.34896200	2.12808700	-0.52940100
H	1.85055600	1.40976000	-1.19048200
H	2.12986900	2.54065900	0.12999200
C	0.74780100	3.23490500	-1.39278400
H	-0.02517200	2.83997700	-2.06352600
H	1.52092700	3.73274100	-1.98829500
H	-0.54412400	3.72151800	0.11367700
H	-0.46652700	4.93692200	-1.07128500
H	0.75051700	4.78952900	0.03711900
N	0.07732400	4.26548100	-0.52661500
O	-0.73024100	2.05126800	0.68416000

7.2.2 $E-1_{sp}-2M_{sc}$

C	0.55824400	-0.63841500	-1.46431600
C	-1.76918800	-0.49393200	-0.43508900
C	-1.81882300	-1.48646700	0.58693500
C	1.88115000	-0.77912500	-0.72084900
C	1.94846800	-1.41089800	0.55556300
H	0.13099200	-1.63134200	-1.65490300
H	0.73982000	-0.15581100	-2.43417000
C	0.67799800	-1.76647100	1.09130600
C	-0.54243900	-1.83902600	1.11120100
C	4.30474700	-0.54656900	-0.67582600
H	5.22278800	-0.20660800	-1.15939600
C	4.36129100	-1.17437500	0.57413700
H	5.32243500	-1.32593500	1.06919600
C	-4.21733900	-1.66584800	0.26315300
C	-4.15865600	-0.71350400	-0.76082300
H	-5.06641500	-0.42014700	-1.29077000
C	3.07281100	-0.34926900	-1.31016000
C	3.18637600	-1.60342500	1.19209600
C	-2.93397800	-0.13645400	-1.11541900
C	-3.05466300	-2.05882500	0.92844100
H	3.03551100	0.14778300	-2.28212900
H	3.21505500	-2.08750500	2.16949300
H	-2.87703500	0.60276300	-1.91641500
H	-3.09056700	-2.81753500	1.71125900
H	-5.17405400	-2.11456600	0.53655300
N	-0.51468700	0.13122700	-0.76185900
C	-0.24627400	1.42076100	-0.43887400

C	-1.21217400	2.15710800	0.48494000
H	-1.21149800	1.64022600	1.45964500
H	-2.24239200	2.09573700	0.11299600
C	-0.86164900	3.63135000	0.64194200
H	-1.52631100	4.11912300	1.36313400
H	-0.92244400	4.15674000	-0.31864000
H	0.69393600	3.41129700	2.05933900
H	0.84115100	4.77686500	1.14087400
H	1.14385600	3.26725500	0.44851300
N	0.55489200	3.79616000	1.12170200
O	0.80354100	1.97128200	-0.82295300

7.2.3 $E-1_{sp}-2_{ap}$

C	-0.90600300	-0.60272400	1.42570300
C	1.44949600	-0.87685000	0.49708900
C	1.34829800	-1.78932400	-0.59507300
C	-2.18940500	-0.41417600	0.62529700
C	-2.32111200	-0.93715000	-0.69481700
H	-0.70770700	-1.67460000	1.55677100
H	-1.03807100	-0.15891500	2.42223900
C	-1.12530800	-1.51586500	-1.20723800
C	0.05419000	-1.83764500	-1.18749100
C	-4.51099700	0.31344700	0.51088700
H	-5.36367100	0.80419900	0.98459900
C	-4.63234100	-0.20980800	-0.78166000
H	-5.57876500	-0.12953300	-1.31995200
C	3.64947900	-2.46425900	-0.21928400
C	3.73564500	-1.59043400	0.87040600
H	4.65985700	-1.52030500	1.44662200
C	-3.29735700	0.21295400	1.20087700
C	-3.53954300	-0.83126300	-1.38683600
C	2.63355700	-0.80776000	1.23304300
C	2.46039800	-2.57243300	-0.94315200
H	-3.20863300	0.62889100	2.20695300
H	-3.61757300	-1.23746700	-2.39651800
H	2.68918400	-0.13194600	2.08822200
H	2.37941500	-3.26795200	-1.77955400
H	4.51008800	-3.07467300	-0.49897100
N	0.33620800	-0.03193600	0.82915300
C	0.37481300	1.32061000	0.64467600
C	1.56822500	1.89332000	-0.11528100
H	1.78085500	1.26466900	-0.99393100
H	2.46345800	1.85318700	0.52424100
C	1.27587300	3.32852100	-0.52859300
H	1.12488200	3.98046100	0.33790900
H	0.39761900	3.39635400	-1.18005700
H	3.30351800	3.88946400	-0.75285700
H	2.26290400	4.85786100	-1.58739600
H	2.62343000	3.35442800	-2.15817300
N	2.43977300	3.89012800	-1.30429700
O	-0.53501300	2.05544600	1.04181900

7.2.4 $E-1P-2_{ap}$

C	-0.97623200	-0.24092300	1.39621000
---	-------------	-------------	------------

C	1.28746800	-0.91140400	0.45803800
C	1.04138300	-2.00968300	-0.41812500
C	-2.27804700	-0.07291100	0.62328300
C	-2.53293500	-0.82814300	-0.55953700
H	-0.86791000	-1.28595600	1.71403500
H	-1.00785200	0.38647300	2.29740700
C	-1.42751200	-1.61815400	-0.98629500
C	-0.28271000	-2.04543400	-0.94128800
C	-4.51864000	0.86389200	0.44438700
H	-5.29120600	1.52748800	0.83813100
C	-4.76251500	0.11147900	-0.71026900
H	-5.72501600	0.18516500	-1.22025900
C	3.29013100	-2.82276900	0.00201300
C	3.51688000	-1.76196000	0.88604200
H	4.47506000	-1.67043400	1.40045200
C	-3.28424800	0.77178200	1.09830900
C	-3.77167100	-0.73132100	-1.21532600
C	2.51225300	-0.81644300	1.12227100
C	2.05658100	-2.95389300	-0.63904700
H	-3.09927700	1.36549000	1.99616500
H	-3.94555800	-1.31791300	-2.11876000
H	2.67783000	0.00822500	1.81775000
H	1.86598200	-3.79058200	-1.31246500
H	4.07473900	-3.55960600	-0.17932200
N	0.27517200	0.08945300	0.65112900
C	0.43293800	1.38987100	0.26254200
C	1.56487000	1.73933200	-0.70064900
H	1.06509200	2.01678500	-1.64375600
H	2.22622000	0.89029100	-0.90797300
C	2.35586800	2.92811000	-0.17090100
H	2.91121700	2.68054200	0.74209300
H	1.70456000	3.78708400	0.02491700
H	4.04069500	2.62217800	-1.40903500
H	3.91858300	4.16829000	-0.84737400
H	2.93459700	3.65438200	-2.06741700
N	3.37580300	3.36953600	-1.18752900
O	-0.35721900	2.27132600	0.61503300

7.2.5 *E-1M-2P_{sc}*

C	0.72567300	-0.07133000	-1.59120300
C	-1.63295200	-0.17437400	-0.65707900
C	-1.67739200	-1.37596400	0.11413000
C	2.02832300	-0.28191300	-0.83221900
C	2.08344300	-1.14835900	0.29952100
H	0.34854100	-1.03429400	-1.95825000
H	0.90921500	0.57567300	-2.45894200
C	0.81087300	-1.66434500	0.68478600
C	-0.40531800	-1.78987500	0.60824200
C	4.42603200	0.06803000	-0.60727800
H	5.34055800	0.54655900	-0.96321900
C	4.46933100	-0.78773100	0.49950100
H	5.41570300	-0.97864600	1.00877700
C	-4.06698800	-1.51727400	-0.27114000
C	-4.01665500	-0.35330200	-1.04604700

H	-4.92585200	0.04032500	-1.50338000
C	3.21388300	0.31884900	-1.26096200
C	3.29937600	-1.39433000	0.95785200
C	-2.80036400	0.30909900	-1.24944600
C	-2.90226100	-2.03445600	0.29960700
H	3.18770500	0.99306700	-2.11939700
H	3.31563400	-2.05834100	1.82334500
H	-2.75474100	1.20858300	-1.86530200
H	-2.93025600	-2.94898500	0.89301300
H	-5.01769400	-2.03057400	-0.11802400
N	-0.39033000	0.52964200	-0.79676200
C	-0.21253500	1.82465600	-0.37422800
C	-1.20728700	2.44434000	0.61198700
H	-2.15046600	2.68321000	0.09984700
H	-0.75188400	3.39819200	0.90879300
C	-1.56369100	1.62899700	1.85669300
H	-2.28801000	0.83304100	1.65915100
H	-1.97509800	2.29196800	2.62654000
H	-0.02299800	0.17242000	1.87300400
H	-0.57672600	0.55820000	3.37589700
H	0.42691500	1.60347700	2.59205500
N	-0.35439000	0.95473700	2.45885500
O	0.77919300	2.46889600	-0.72060700

7.2.6 *E-1M-2M_{sc}*

C	0.66109900	-0.34406100	-1.59992200
C	-1.68902000	-0.25695500	-0.63503200
C	-1.75365100	-1.31124600	0.32488600
C	1.96652600	-0.47006800	-0.82566800
C	2.01283600	-1.14325400	0.43073300
H	0.26082100	-1.34134300	-1.82218200
H	0.85208200	0.16677800	-2.55282900
C	0.73369400	-1.55591100	0.90657700
C	-0.48522900	-1.67280600	0.86753000
C	4.37624200	-0.15950200	-0.68171500
H	5.29868100	0.22834700	-1.11844000
C	4.41068300	-0.82650500	0.54851300
H	5.35817800	-0.96122400	1.07341900
C	-4.14500700	-1.47924800	-0.04013000
C	-4.07417300	-0.46476400	-1.00201700
H	-4.97609300	-0.14082600	-1.52398200
C	3.16269700	0.01881900	-1.35588200
C	3.23066900	-1.31600100	1.10897100
C	-2.84813700	0.13661200	-1.30658000
C	-2.99031000	-1.90878100	0.61585700
H	3.14317400	0.54769600	-2.31109100
H	3.24027100	-1.83287200	2.06970300
H	-2.78577600	0.92538800	-2.05810200
H	-3.03264600	-2.71225300	1.35208800
H	-5.10380200	-1.94594500	0.19168300
N	-0.43362600	0.39121900	-0.89516900
C	-0.20761900	1.71989000	-0.63561300
C	-1.14486400	2.45823700	0.31641600
H	-2.15527700	2.03550000	0.36783700
H	-1.22779100	3.48950000	-0.05004500

C	-0.52499200	2.52192500	1.71203800
H	-1.07033800	3.22465200	2.35225500
H	0.53131000	2.81387300	1.67155900
H	-1.54950100	0.88610800	2.56868800
H	-0.11795600	1.21534300	3.31376200
H	-0.12987800	0.42456600	1.86386300
N	-0.58253500	1.18022800	2.40238800
O	0.80362700	2.28728600	-1.05406300

7.2.7 *E-1M-2_{ap}*

C	0.88878300	-0.80242000	-1.40356300
C	-1.51481100	-0.65389700	-0.58946300
C	-1.55648900	-1.35403300	0.65313700
C	2.15023700	-0.57657500	-0.57937000
C	2.17071700	-0.83668900	0.82271700
H	0.58100200	-1.85352900	-1.32891600
H	1.10463000	-0.58588500	-2.45870800
C	0.90103800	-1.19337100	1.36017000
C	-0.30191000	-1.41198900	1.32558400
C	4.52444100	-0.04852900	-0.46116700
H	5.44174000	0.26157400	-0.96577300
C	4.53576100	-0.31363700	0.91313100
H	5.46061700	-0.21194700	1.48420400
C	-3.89780500	-1.86507600	0.26679000
C	-3.84494500	-1.20589000	-0.96706700
H	-4.73124600	-1.15689500	-1.60197400
C	3.33890600	-0.17589800	-1.19434200
C	3.36111500	-0.70376200	1.55712600
C	-2.65303400	-0.61305100	-1.39776600
C	-2.75865100	-1.94893800	1.06925000
H	3.33636800	0.03896700	-2.26520100
H	3.35346300	-0.90693400	2.62910100
H	-2.60168400	-0.10271300	-2.36118000
H	-2.78570800	-2.48114200	2.02095900
H	-4.82867100	-2.32823000	0.59892200
N	-0.30442300	0.00083400	-1.00293700
C	-0.19445200	1.36163000	-1.10662000
C	-1.27524100	2.22283700	-0.45453100
H	-2.28430100	1.83393900	-0.63953800
H	-1.19590400	3.22407000	-0.89819300
C	-1.00893100	2.28584300	1.04866500
H	-0.03059100	2.73087600	1.26738800
H	-1.06330400	1.29733600	1.51937400
H	-2.03104800	4.10586900	1.36819900
H	-1.87158300	3.19854100	2.73751800
H	-2.98700000	2.77895100	1.59751900
N	-2.03988400	3.14686000	1.72872900
O	0.79437400	1.89049300	-1.62004100

7.2.8 *Z-1_{sp}-2P_{sc}*

C	-1.70025100	-0.91756500	0.71517300
C	-0.40314100	-0.50416400	1.40328700
C	0.84098000	-1.93040300	-0.95992400

C	2.06790200	-1.37935900	-0.48978600
C	1.90288800	-0.25549900	0.36684100
H	0.14098700	-1.40463900	1.71585900
H	-0.63477000	0.05803500	2.31962000
C	-1.68639900	-1.71625400	-0.46677600
C	-0.37976300	-1.99336900	-0.96126900
C	3.35901100	-1.87475200	-0.73424500
C	3.01323200	0.32986400	0.97207000
C	4.46512500	-1.26835500	-0.13684700
C	4.29407200	-0.17299400	0.71809900
H	5.15990700	0.29360300	1.19127000
H	5.46611300	-1.65765700	-0.33166400
H	3.48200000	-2.73964900	-1.38739900
C	-2.89021300	-2.14333800	-1.04937500
H	-2.85890900	-2.75158900	-1.95453200
C	-4.11035000	-1.79101200	-0.46933000
H	-5.04440600	-2.12556900	-0.92460200
C	-4.13411800	-1.01200500	0.69182200
H	-5.08667600	-0.73743800	1.14891400
C	-2.93579800	-0.57963500	1.27353600
H	-2.96668000	0.02932400	2.18032100
C	0.29403400	1.49397500	0.05219700
C	-1.06615700	2.11798800	0.34263200
H	-1.82556500	1.60689600	-0.27086000
C	-1.08524300	3.62090900	0.08146500
H	-2.07843600	4.03954400	0.27539700
H	-0.34644500	4.14206500	0.70206900
N	0.58209400	0.28321100	0.59709300
N	-0.72013000	3.91062500	-1.34771600
H	-0.60169600	4.91044900	-1.52123500
H	0.17745500	3.40565400	-1.50867700
O	1.10281700	2.09079200	-0.68685300
H	-1.36116600	1.95817900	1.38794800
H	2.86945600	1.18622100	1.63238500
H	-1.42231600	3.55918600	-2.00305300

7.2.9 $Z-1_{sp}-2M_{sc}$

C	-1.80916600	-0.77395200	0.68323200
C	-0.49176400	-0.38059700	1.34687000
C	0.66291100	-2.08249100	-0.88428300
C	1.92330800	-1.58842700	-0.44186800
C	1.83716100	-0.39508500	0.32715400
H	-0.01593400	-1.28128500	1.75566000
H	-0.70022500	0.28172400	2.19918500
C	-1.84553700	-1.66776500	-0.42749800
C	-0.55901900	-2.06383400	-0.89128800
C	3.17455500	-2.19871800	-0.62979700
C	2.98456500	0.14311800	0.90816200
C	4.31856000	-1.63848100	-0.06021700
C	4.22420800	-0.47464500	0.71250100
H	5.11839900	-0.04418900	1.16685800
H	5.28797800	-2.11703500	-0.21084600
H	3.23539300	-3.11624400	-1.21650600
C	-3.07370100	-2.07565000	-0.97170300

H	-3.07957600	-2.75791100	-1.82301500
C	-4.27027700	-1.61145800	-0.42218600
H	-5.22316600	-1.93165000	-0.84778200
C	-4.24624600	-0.73924100	0.67041500
H	-5.18010700	-0.37692300	1.10433300
C	-3.02317300	-0.32613200	1.21366300
H	-3.01500800	0.35527100	2.06804700
C	0.40721300	1.48906000	-0.06690000
C	-0.85817200	2.27594700	0.24989000
H	-1.74864400	1.64372300	0.14755000
C	-1.04898700	3.47780900	-0.66732200
H	-1.14010400	3.16150400	-1.71331500
H	-1.93954400	4.04970900	-0.38515500
N	0.56083000	0.26106700	0.49666700
N	0.14135300	4.39437600	-0.60712900
H	0.08706800	5.14161100	-1.30220200
H	0.25106300	4.82829600	0.31250700
O	1.28280600	1.99158000	-0.79882200
H	-0.82165700	2.58573900	1.30869800
H	2.90277400	1.05318400	1.50396600
H	0.96492600	3.78699000	-0.79712400

7.2.10 $E-1_{sp}-2P_{sc}$ (water)

C	-0.62402200	-0.52576100	1.43912600
C	1.71450100	-0.55510500	0.42507800
C	1.72836800	-1.64758300	-0.49123800
C	-1.94689400	-0.67506800	0.69884600
C	-2.03381500	-1.42656000	-0.50970800
H	-0.23899000	-1.51533000	1.71649300
H	-0.78984300	0.04585900	2.36226900
C	-0.77535200	-1.88681700	-0.99148400
C	0.44173200	-2.00377000	-0.98626700
C	-4.35654000	-0.33953600	0.60331800
H	-5.26143100	0.08802600	1.03985500
C	-4.43289200	-1.08554200	-0.57860000
H	-5.39648000	-1.24209100	-1.06732400
C	4.12109300	-1.87120200	-0.15036800
C	4.09698300	-0.81722700	0.76955200
H	5.01557700	-0.50002700	1.26601700
C	-3.12145000	-0.13591000	1.22964300
C	-3.27465400	-1.62646000	-1.13781300
C	2.89289700	-0.16735100	1.06382700
C	2.94353100	-2.29225000	-0.77143700
H	-3.06842900	0.45219100	2.14853500
H	-3.31878800	-2.20343100	-2.06279300
H	2.86486800	0.64845900	1.78803600
H	2.95210900	-3.12717600	-1.47323000
H	5.06170500	-2.37662200	-0.37656400
N	0.48276900	0.14086200	0.68570700
C	0.29733100	1.43464200	0.32691500
C	1.35250000	2.12526500	-0.53164600
H	1.84983300	1.40604100	-1.19501600
H	2.13636700	2.53267200	0.12746400
C	0.75541700	3.23671400	-1.39167100
H	-0.02182200	2.84745100	-2.06072200

H	1.52985800	3.73048400	-1.98874200
H	-0.53205700	3.73197500	0.11618200
H	-0.44415200	4.94792100	-1.06563400
H	0.77193900	4.78761300	0.04180900
N	0.09405000	4.27049900	-0.52272300
O	-0.72755100	2.05294700	0.68075700

7.3 Azides

7.3.1 Phenyl Azide (MeCN)

N	-1.47523800	-0.88765200	-0.00011600
N	-3.37275900	0.53580100	0.00020700
N	-2.41950700	-0.09088700	-0.00008600
C	-0.14721200	-0.36455100	-0.00005100
C	0.88476300	-1.31384500	0.00002100
C	0.14807500	1.00740300	-0.00007700
C	2.21364800	-0.88647400	0.00006900
H	0.63337900	-2.37573600	0.00003500
C	1.48283600	1.42026900	-0.00002600
H	-0.65480900	1.74757500	-0.00014300
C	2.51928400	0.47996400	0.00004800
H	3.01508800	-1.62809700	0.00012600
H	1.71088100	2.48822100	-0.00004700
H	3.55963200	0.81061200	0.00008700

7.3.2 Phenyl Azide (water)

N	-1.47523800	-0.88765200	-0.00011600
N	-3.37275900	0.53580100	0.00020700
N	-2.41950700	-0.09088700	-0.00008600
C	-0.14721200	-0.36455100	-0.00005100
C	0.88476300	-1.31384500	0.00002100
C	0.14807500	1.00740300	-0.00007700
C	2.21364800	-0.88647400	0.00006900
H	0.63337900	-2.37573600	0.00003500
C	1.48283600	1.42026900	-0.00002600
H	-0.65480900	1.74757500	-0.00014300
C	2.51928400	0.47996400	0.00004800
H	3.01508800	-1.62809700	0.00012600
H	1.71088100	2.48822100	-0.00004700
H	3.55963200	0.81061200	0.00008700

7.3.3 Methyl Azide (MeCN)

C	1.55169300	0.28721500	0.00000800
H	1.55383500	0.92221600	-0.90023100
H	1.55368000	0.92262900	0.89995100
H	2.44973300	-0.34087900	0.00023200
N	0.39131700	-0.63570600	0.00006900
N	-1.79739400	0.27608800	0.00008000
N	-0.71783900	-0.10141800	-0.00014800

8 Coordinates of Transition States

8.1 Phenyl Azide (PhN₃) + Non-Protonated Cyclooctyne

8.1.1 *E-1M-2M_{sc}-anti-11*

C	-1.83692600	1.21642900	-1.61101300
C	-2.86960100	-0.81253700	-0.52964500
C	-1.81929600	-1.76592800	-0.41561600
C	-0.57313300	1.91686900	-1.15333900
C	0.46601100	1.17780100	-0.52163000
H	-1.59713800	0.40906500	-2.31469600
H	-2.49793900	1.93113200	-2.12006900
C	0.24349500	-0.22963100	-0.36791900
C	-0.47206000	-1.25558000	-0.34373000
N	2.38318600	-1.27311400	-0.48395100
N	1.88416700	-2.40654100	-0.27523600
N	0.84462900	-2.93726400	-0.19857800
C	0.73945300	3.94855600	-0.87349800
H	0.84527600	5.02542000	-1.01971200
C	1.74281300	3.22448500	-0.21902200
H	2.63527800	3.73139800	0.15308800
C	-3.47883900	-3.54749500	-0.54202600
C	-4.50181100	-2.60386100	-0.68078700
H	-5.53942600	-2.92428900	-0.79035400
C	-0.41216200	3.29467800	-1.32175600
C	1.60614400	1.84834700	-0.04177300
C	-4.19124800	-1.24197600	-0.68691600
C	-2.15206000	-3.13325100	-0.42060200
H	-1.21202500	3.86370700	-1.79962500
H	2.37927200	1.28180900	0.47291500
H	-4.97653600	-0.49226200	-0.79780800
H	-1.35653000	-3.86985000	-0.33066600
H	-3.71260300	-4.61374900	-0.53883800
N	-2.58595800	0.58805600	-0.48927900
C	-3.12060000	1.43165400	0.45737200
C	-3.62775700	0.84973300	1.76441200
H	-3.78040200	-0.23513800	1.71670500
H	-4.59459200	1.32562700	1.98886500
C	-2.62433200	1.17339200	2.89679700
H	-3.06172100	0.82711100	3.84629600
H	-2.50474000	2.26500200	2.97232800
H	-0.83097000	0.92964200	1.91670300
H	-1.37308400	-0.43260400	2.61128100
N	-1.29296200	0.57382300	2.75174500
O	-3.07491200	2.65728400	0.29880300
C	3.72248400	-0.99106000	-0.11411700
C	4.37724900	-1.65070200	0.94021000
C	4.37501700	0.03194200	-0.81902300
C	5.68237700	-1.28670500	1.27494500
H	3.86309500	-2.44388300	1.48651500
C	5.67505400	0.39794300	-0.46381900
H	3.85253000	0.53372000	-1.63449400
C	6.33454900	-0.25968400	0.58077700
H	6.19116800	-1.80663700	2.08948400
H	6.17697700	1.19687500	-1.01336300
H	7.35304300	0.02440000	0.85240300

8.1.2 E-1M-2M_{sc}-syn-11

C	-2.12786700	1.82604700	-0.99706700
C	-3.01720000	-0.42890900	-0.38072600
C	-2.11222900	-1.39188100	-0.90034400
C	-0.67941600	2.28180800	-0.97349800
C	0.40135100	1.35588000	-1.02320300
H	-2.33723900	1.34313100	-1.96116200
H	-2.78203200	2.70529700	-0.91385000
C	0.06366800	-0.03463000	-0.94651900
C	-0.72815300	-1.00210600	-0.95406200
N	1.95219500	-1.18457200	-0.06653900
N	1.39378400	-2.30255600	-0.18579400
N	0.35280500	-2.75660800	-0.47558600
C	0.92580700	4.11285300	-1.11665900
H	1.12320000	5.18642200	-1.14248000
C	1.98097900	3.19857800	-1.20362500
H	3.00979500	3.54928200	-1.30513400
C	-3.97386100	-2.91836300	-1.23377800
C	-4.86179500	-1.96171400	-0.72764700
H	-5.92902400	-2.18102900	-0.66236800
C	-0.38843900	3.64924600	-1.00519400
C	1.71891500	1.83052400	-1.15534500
C	-4.38241900	-0.71655600	-0.31015700
C	-2.60948100	-2.63785100	-1.31894300
H	-1.21254300	4.36404600	-0.94839500
H	2.53362000	1.11378800	-1.22986500
H	-5.06172300	0.04209400	0.08213100
H	-1.91477900	-3.37941500	-1.71273500
H	-4.34700100	-3.88923200	-1.56535000
N	-2.52278400	0.84633300	0.04268100
C	-2.47330400	1.25118300	1.35174900
C	-2.70562400	0.23256000	2.45358900
H	-3.07728300	-0.72600100	2.07032300
H	-3.47285400	0.65248100	3.12341500
C	-1.40807700	-0.00089500	3.25967100
H	-1.66133600	-0.61755600	4.13636500
H	-1.04190800	0.96589900	3.63788300
H	-0.63347900	-1.53804000	2.13556500
H	-0.00984200	-0.09323200	1.74380900
N	-0.31419900	-0.65665700	2.53578100
O	-2.17039500	2.41812600	1.63301900
C	3.35582700	-1.07987400	0.10625700
C	4.26041100	-1.98826900	-0.46898100
C	3.82808900	0.01303800	0.84844200
C	5.63176500	-1.80091900	-0.28809800
H	3.88402800	-2.83322000	-1.04874600
C	5.20316000	0.19820400	1.00914700
H	3.11124900	0.70669500	1.28984200
C	6.10915300	-0.70691500	0.44490900
H	6.33261100	-2.51265600	-0.72957700
H	5.56625200	1.05088700	1.58646600
H	7.18326000	-0.56247100	0.57640600

8.1.3 $E-1M-2M_{sc}-syn-12$

C	2.69602400	0.87989900	-1.22189900
C	0.51604600	1.98749700	-0.72144900
C	-0.47252500	1.01317100	-1.01683100
C	3.11930500	-0.53857900	-0.87918100
C	2.17718200	-1.58460700	-0.66202600
H	2.15813600	0.87676500	-2.17939900
H	3.59500500	1.49976600	-1.34633000
C	0.77911100	-1.22577900	-0.62055100
C	-0.09365800	-0.34558900	-0.78108000
N	-0.27110700	-2.86523700	0.38142900
N	-1.30609800	-2.35009300	0.54874400
N	-1.86753400	-1.23303500	0.41484100
C	4.93042900	-2.16048000	-0.66873000
H	6.00098000	-2.37554300	-0.66813600
C	4.00240800	-3.18860900	-0.47625900
H	4.34026500	-4.21617600	-0.32763400
C	-1.96666300	2.78595500	-1.74087000
C	-0.99103900	3.74316000	-1.43596900
H	-1.19300200	4.80380500	-1.59608000
C	4.48270900	-0.85080900	-0.86393500
C	2.63784800	-2.90059200	-0.46507600
C	0.25377000	3.34165800	-0.94165800
C	-1.70930700	1.43012600	-1.53820000
H	5.20777100	-0.04787000	-1.01511800
H	1.91292200	-3.69662800	-0.30533400
H	1.03138600	4.07432800	-0.71926900
H	-2.46374800	0.68187900	-1.77794400
H	-2.93351000	3.09786900	-2.14008400
N	1.79664900	1.55388800	-0.25260700
C	2.27898500	1.81015900	1.00446600
C	1.31862300	2.30129600	2.07333700
H	0.34571400	2.59422500	1.65977100
H	1.77285500	3.18778800	2.54333400
C	1.11412900	1.20718000	3.14600300
H	0.49289200	1.63189800	3.95004900
H	2.08937000	0.95297600	3.58883500
H	-0.40506300	0.16391500	2.22073700
H	1.06074900	-0.47402000	1.96283600
N	0.48508700	-0.03234400	2.67772400
O	3.45748500	1.55715100	1.28688200
C	-3.27285500	-1.11813700	0.30054200
C	-4.08938900	-2.15128100	-0.19016200
C	-3.83162200	0.12072100	0.65039700
C	-5.46258100	-1.93837700	-0.31866800
H	-3.64567600	-3.11109500	-0.46171100
C	-5.20452800	0.32669600	0.50032700
H	-3.18100900	0.91050100	1.02770500
C	-6.02458800	-0.70022300	0.01913000
H	-6.09751100	-2.74491100	-0.69128300
H	-5.63552300	1.29314700	0.76924300
H	-7.09875400	-0.53880700	-0.09009900

8.1.4 $Z-1_{sp}-2M_{sc}-syn-12$

C	-2.33573500	-0.04146200	-1.46498000
---	-------------	-------------	-------------

C	-0.56301000	-1.68492100	-0.85794500
C	0.63913600	-0.93317000	-0.86741000
C	-2.51039700	1.38613800	-0.97391000
C	-1.42656100	2.14442500	-0.44614900
H	-1.63324300	-0.04057500	-2.30909400
H	-3.29477700	-0.40859200	-1.85980900
C	-0.15541500	1.47472200	-0.29101500
C	0.52096900	0.44100200	-0.48293800
N	1.14444600	2.80537500	0.82899200
N	2.07158700	2.10871400	0.97233700
N	2.43973300	0.92383600	0.77366200
C	-3.95837400	3.33889900	-0.76233300
H	-4.94275800	3.79437500	-0.88679300
C	-2.89243700	4.08296900	-0.25052300
H	-3.03424300	5.12874100	0.02937000
C	1.82471300	-2.89318400	-1.67889500
C	0.63732500	-3.63546100	-1.64169600
H	0.63669900	-4.68624600	-1.93756500
C	-3.75877600	2.00088000	-1.11607900
C	-1.63943600	3.48936500	-0.09097600
C	-0.55567100	-3.02659400	-1.24271200
C	1.82606300	-1.55137200	-1.30054900
H	-4.59296000	1.41902100	-1.51557700
H	-0.81023200	4.06888500	0.30926400
H	-1.49298300	-3.58438000	-1.22935600
H	2.74426100	-0.96796500	-1.33980400
H	2.75412500	-3.36214100	-2.00746500
N	-1.79280200	-1.03606700	-0.50384600
C	-2.42594600	-1.40656800	0.65697600
C	-3.78766200	-0.79265900	0.94421000
H	-4.41178200	-0.82136000	0.03589900
H	-3.64095900	0.27548400	1.17572300
C	-4.51465300	-1.48587000	2.10211500
H	-5.43438800	-0.91991000	2.31696600
H	-3.88756600	-1.43770200	3.00441600
H	-5.46667700	-2.96622300	1.04371200
H	-4.03261900	-3.42212900	1.67153500
N	-4.87822100	-2.89056200	1.87282300
O	-1.90467500	-2.20766800	1.44340800
C	3.81477600	0.59310300	0.68477200
C	4.79453200	1.50910600	0.26472600
C	4.16849600	-0.73147200	0.98408300
C	6.12241600	1.09387400	0.15570300
H	4.51150200	2.53718300	0.03049700
C	5.49785800	-1.13910100	0.85453100
H	3.39487800	-1.42857100	1.30835300
C	6.47911400	-0.22996400	0.44317300
H	6.88333400	1.80958000	-0.16262700
H	5.76787500	-2.17167400	1.08483800
H	7.51875600	-0.54963200	0.34939700

8.1.5 *E-1M-2M_{sc}-syn-12 (water)*

C	2.69652100	0.88050200	-1.22110800
C	0.51599000	1.98742300	-0.72150500
C	-0.47230900	1.01284400	-1.01685600

C	3.11991400	-0.53807700	-0.87883600
C	2.17795100	-1.58421200	-0.66140600
H	2.15910100	0.87770100	-2.17885700
H	3.59540200	1.50061300	-1.34496600
C	0.77982800	-1.22564000	-0.61963600
C	-0.09315700	-0.34574000	-0.78049000
N	-0.27028000	-2.86526900	0.38351500
N	-1.30539100	-2.35003500	0.55004000
N	-1.86706300	-1.23331700	0.41529200
C	4.93128300	-2.15999900	-0.66972000
H	6.00183700	-2.37504000	-0.66994600
C	4.00340900	-3.18819200	-0.47676100
H	4.34138900	-4.21577000	-0.32850700
C	-1.96632500	2.78511800	-1.74224200
C	-0.99089400	3.74254800	-1.43743000
H	-1.19290200	4.80309000	-1.59810500
C	4.48335800	-0.85031200	-0.86451400
C	2.63883100	-2.90019700	-0.46483100
C	0.25378000	3.34144300	-0.94241200
C	-1.70895200	1.42939200	-1.53884700
H	5.20833600	-0.04739900	-1.01633800
H	1.91402500	-3.69633300	-0.30496400
H	1.03119700	4.07431900	-0.72005200
H	-2.46324000	0.68099100	-1.77858100
H	-2.93304100	3.09677700	-2.14195000
N	1.79654100	1.55399700	-0.25198900
C	2.27777700	1.80990700	1.00532900
C	1.31695900	2.30180600	2.07342500
H	0.34447300	2.59510000	1.65919200
H	1.77129300	3.18829100	2.54332900
C	1.11127100	1.20831400	3.14640100
H	0.48990300	1.63369000	3.94995900
H	2.08610600	0.95356500	3.58985300
H	-0.40898900	0.16605400	2.22208500
H	1.05617800	-0.47197500	1.96201200
N	0.48149000	-0.03097500	2.67813600
O	3.45608000	1.55627900	1.28890700
C	-3.27239500	-1.11851400	0.30038800
C	-4.08852400	-2.15180800	-0.19065200
C	-3.83135400	0.12034500	0.64989500
C	-5.46168500	-1.93903800	-0.31980800
H	-3.64458200	-3.11157200	-0.46200400
C	-5.20422600	0.32617100	0.49917100
H	-3.18100700	0.91027000	1.02736400
C	-6.02394200	-0.70089000	0.01766700
H	-6.09636800	-2.74563400	-0.69269900
H	-5.63542700	1.29262100	0.76772700
H	-7.09806300	-0.53956600	-0.09212000

8.2 Phenyl Azide (PhN₃) + Protonated Cyclooctyne

8.2.1 *E*-1_{sp}-2P_{sc}-anti-11

C	1.65462500	-0.75863300	-1.81120500
C	2.57121300	1.25770400	-0.57961200
C	1.44938100	2.07858700	-0.28031000
C	0.48691400	-1.61377600	-1.36272600

C	-0.56401600	-1.04825200	-0.58953600
H	1.30892000	0.08748000	-2.41821200
H	2.34742800	-1.35686000	-2.41849900
C	-0.45163200	0.34646500	-0.28189800
C	0.16517000	1.43026000	-0.17911500
N	-2.67471600	1.18694100	-0.19640100
N	-2.27396100	2.33439300	0.11891300
N	-1.28258700	2.94849400	0.21555600
C	-0.63316600	-3.77274200	-1.26293500
H	-0.66066000	-4.82979800	-1.53493600
C	-1.64745200	-3.22149200	-0.47127700
H	-2.46941800	-3.84567100	-0.11540700
C	2.92589200	4.01791800	-0.32496500
C	4.01540200	3.20337600	-0.64786000
H	5.00574500	3.63618700	-0.79852600
C	0.42961500	-2.97128800	-1.68974300
C	-1.61187900	-1.86937000	-0.13473500
C	3.83123500	1.82500300	-0.78424200
C	1.65653000	3.46415100	-0.15227500
H	1.23971700	-3.40777300	-2.27764000
H	-2.39339100	-1.43801700	0.48721400
H	4.66818800	1.17490300	-1.04422800
H	0.80877300	4.10498100	0.08010600
H	3.06109200	5.09562200	-0.21679300
N	2.41840700	-0.16469800	-0.67618700
C	3.04667200	-1.01383900	0.17442300
C	3.71717000	-0.45168200	1.42392300
H	3.26224100	0.50052900	1.72368100
H	4.77325900	-0.23713700	1.19236400
C	3.61854800	-1.41857500	2.60276200
H	2.57182800	-1.64484700	2.84087300
H	4.10738200	-1.00562900	3.49198900
H	3.89685100	-2.99410400	1.32696400
H	4.06957000	-3.45429800	2.95391500
H	5.29244800	-2.64220000	2.19506400
N	4.27586400	-2.72897800	2.26461400
O	3.05700200	-2.24283800	-0.04143600
C	-3.97121000	0.74250400	0.16634600
C	-4.65142800	1.22075300	1.29933200
C	-4.54878400	-0.25390900	-0.63528400
C	-5.90876900	0.70407300	1.61576800
H	-4.19429000	1.99421000	1.91948400
C	-5.80022400	-0.77430400	-0.29882000
H	-4.00689000	-0.61341300	-1.51092400
C	-6.48580200	-0.29710800	0.82405300
H	-6.43886800	1.08347900	2.49190600
H	-6.24420000	-1.55168000	-0.92390500
H	-7.46682100	-0.70126300	1.08111400

8.2.2 *E-1_{sp}-2P_{sc}-syn-11*

C	-1.96726100	1.09134200	-1.72079800
C	-2.74263000	-1.00911500	-0.57845300
C	-1.66797600	-1.93415000	-0.63518100
C	-0.59850200	1.73717100	-1.61178900

C	0.55488700	1.00109200	-1.21550800
H	-1.95233400	0.33036100	-2.51216900
H	-2.70777700	1.85296100	-2.00168400
C	0.34837500	-0.34929800	-0.77893000
C	-0.33827000	-1.38123200	-0.60527800
N	2.26908200	-1.05438900	0.47605800
N	1.80927100	-2.21843500	0.58714400
N	0.83039600	-2.82123700	0.35880800
C	0.81651800	3.67496700	-2.04738100
H	0.90961100	4.71613400	-2.36243200
C	1.95151900	2.93810800	-1.69535200
H	2.94241200	3.39414400	-1.73859200
C	-3.29083900	-3.74088900	-0.75940000
C	-4.34264700	-2.81957800	-0.70576400
H	-5.37838800	-3.16197700	-0.73532700
C	-0.44295900	3.06983700	-2.00527800
C	1.81950500	1.61344300	-1.28219200
C	-4.06552600	-1.45170400	-0.62336800
C	-1.96523100	-3.30511000	-0.72360500
H	-1.32857600	3.64119900	-2.29263700
H	2.70104100	1.03612000	-1.01693200
H	-4.87296900	-0.71815300	-0.59566100
H	-1.14697400	-4.02275500	-0.76791400
H	-3.50415600	-4.80903200	-0.83108800
N	-2.45589800	0.39433000	-0.50427800
C	-2.66909000	1.12654500	0.61386400
C	-3.08658200	0.40099900	1.88842400
H	-2.63656600	-0.59954400	1.93264000
H	-4.17841200	0.24918900	1.86800500
C	-2.67685200	1.16565100	3.14352300
H	-1.59136900	1.31933500	3.17667900
H	-2.99301100	0.63630500	4.04876800
H	-3.07256400	2.94756300	2.22091100
H	-2.93839900	3.12214000	3.90296200
H	-4.31902200	2.49042800	3.24949100
N	-3.30189800	2.53384000	3.15079700
O	-2.52024500	2.36528700	0.60807800
C	3.66373600	-0.81626800	0.60163700
C	4.62998000	-1.74974100	0.18987900
C	4.05934200	0.42721200	1.11701100
C	5.98481200	-1.43526900	0.30654000
H	4.31411000	-2.71364700	-0.21377600
C	5.41794800	0.73704500	1.21343100
H	3.29700500	1.13938700	1.43625500
C	6.38465700	-0.19153500	0.81185400
H	6.73356500	-2.16604700	-0.00635100
H	5.72063800	1.70672100	1.61373600
H	7.44594500	0.05098500	0.89350300

8.2.3 *E-1_{sp}-2P_{sc}-syn-12*

C	2.42892700	0.01455100	-1.62868500
C	0.55476900	1.60271100	-1.12552900
C	-0.60427000	0.78724300	-1.04887800
C	2.68921500	-1.34010700	-0.99674000

C	1.64986300	-2.11569200	-0.40830200
H	1.73565300	-0.09705800	-2.47239100
H	3.37213000	0.41990600	-2.02031400
C	0.34077700	-1.51323600	-0.30158100
C	-0.40489500	-0.54179400	-0.55648900
N	-0.86740800	-2.81658900	0.95413300
N	-1.82138000	-2.15142800	1.06627500
N	-2.24510600	-1.00289800	0.78340800
C	4.25680900	-3.16496800	-0.59623700
H	5.27040800	-3.56421300	-0.66933800
C	3.23231400	-3.93228400	-0.03420500
H	3.43676400	-4.93930100	0.33481400
C	-1.90072700	2.61688200	-1.98728600
C	-0.75431300	3.41796700	-2.04301900
H	-0.81279900	4.43806900	-2.42619300
C	3.97793400	-1.87893900	-1.06704100
C	1.94294400	-3.40967200	0.06395000
C	0.47736200	2.90284200	-1.62713100
C	-1.82721300	1.31098200	-1.50199300
H	4.77719600	-1.27710000	-1.50534300
H	1.14777000	-4.00365300	0.50930900
H	1.38628100	3.50269800	-1.69741700
H	-2.71606300	0.68363200	-1.47417500
H	-2.85972800	3.01023200	-2.32933100
N	1.81826200	1.04305800	-0.74392900
C	2.51609500	1.46365000	0.33613600
C	1.85130400	2.45187100	1.28897000
H	0.77074000	2.26461700	1.34850000
H	1.96650500	3.47027200	0.88347400
C	2.43106300	2.37084200	2.69810600
H	2.31157700	1.36556900	3.12017600
H	1.95425900	3.09910800	3.36287100
H	4.29716500	2.01157700	1.94247400
H	4.35423900	2.47593400	3.57381000
H	4.11075900	3.61612500	2.40261800
N	3.90888500	2.64985400	2.67075300
O	3.67119400	1.04692200	0.55664700
C	-3.63364500	-0.73423900	0.69260100
C	-4.57851800	-1.71268800	0.33940900
C	-4.03690500	0.59122100	0.91452600
C	-5.92265900	-1.35722800	0.21827300
H	-4.25592800	-2.74108400	0.16557800
C	-5.38223900	0.93780700	0.77324700
H	-3.28876300	1.33662300	1.18715400
C	-6.32907500	-0.03299700	0.42757200
H	-6.65708100	-2.12014100	-0.04821000
H	-5.69172600	1.97113100	0.94211100
H	-7.38117900	0.23936400	0.32412200

8.2.4 *Z-1_{sp}-2P_{sc}-anti-11*

C	1.79396500	-0.62798700	-1.71613400
C	2.57499000	1.41120900	-0.45705900
C	1.41901000	2.19618500	-0.21251300
C	0.60190400	-1.50419600	-1.38191800

C	-0.49116600	-0.98527100	-0.63286400
H	1.47649700	0.22263800	-2.33281900
H	2.52993900	-1.19325600	-2.30612700
C	-0.42547100	0.40139600	-0.27434800
C	0.15589000	1.50098600	-0.13598900
N	-2.67485800	1.17255900	-0.16181000
N	-2.30450700	2.31695500	0.19908300
N	-1.32677900	2.94934700	0.32010800
C	-0.50458300	-3.67314900	-1.45685600
H	-0.51204700	-4.71181000	-1.79247200
C	-1.54964100	-3.17583300	-0.67216500
H	-2.37721600	-3.82512000	-0.38029700
C	2.82190100	4.18658400	-0.27970300
C	3.95044400	3.40093200	-0.53744700
H	4.92935900	3.86533200	-0.66883600
C	0.56618200	-2.83928000	-1.79492900
C	-1.54275500	-1.84203100	-0.26405000
C	3.82164700	2.01292300	-0.62905700
C	1.56904200	3.59287900	-0.12449000
H	1.39822300	-3.23864300	-2.37984200
H	-2.35426900	-1.45352800	0.34686700
H	4.68923300	1.38167700	-0.82609500
H	0.69125300	4.20887300	0.05824800
H	2.91514500	5.27181700	-0.20775300
N	2.47161300	-0.02291000	-0.53228800
C	3.02358700	-0.74809500	0.47663200
C	3.03623100	-2.26788600	0.36683600
H	3.26376800	-2.58878700	-0.65823000
H	2.02590700	-2.64581800	0.58921700
C	4.06238500	-2.91029400	1.29452100
H	5.07628300	-2.55402800	1.07715400
H	4.03677600	-4.00184300	1.20904800
H	3.71604300	-1.50183300	2.73223200
H	4.51327700	-2.85813900	3.35910600
H	2.89082900	-2.93082600	3.05241900
N	3.77810700	-2.54158300	2.72404400
O	3.50287500	-0.19845400	1.48841700
C	-3.96397200	0.68570400	0.17429700
C	-4.65044500	1.08707000	1.33300600
C	-4.52573200	-0.27329900	-0.68217500
C	-5.89825700	0.53172800	1.62038300
H	-4.20505600	1.83137300	1.99588300
C	-5.76733800	-0.83382400	-0.37493600
H	-3.97967300	-0.57257500	-1.57773600
C	-6.45907600	-0.43308800	0.77371000
H	-6.43339800	0.85152000	2.51701100
H	-6.19893000	-1.58185000	-1.04301100
H	-7.43241600	-0.86829900	1.00823800

8.2.5 *E-1_{sp}-2M_{sc}-syn-11*

C	-2.08523200	2.13000500	-0.49680100
C	-3.10616100	-0.16058000	-0.26374100
C	-2.38419200	-1.09499200	-1.05421300
C	-0.60500700	2.41563600	-0.72249900

C	0.34320200	1.40902600	-1.06129800
H	-2.57665600	1.95823700	-1.46388100
H	-2.55301300	3.01452400	-0.04262300
C	-0.10421900	0.04858000	-1.07590600
C	-0.96859600	-0.85244400	-1.15017200
N	1.56910200	-1.24598100	0.03381500
N	0.94549300	-2.32894400	-0.19826400
N	-0.09769100	-2.68013700	-0.59078100
C	1.14793500	4.09338800	-0.98884400
H	1.45392600	5.14077800	-0.95149400
C	2.06781600	3.10227400	-1.34716700
H	3.09748500	3.36592300	-1.59530600
C	-4.44263900	-2.32109200	-1.42707500
C	-5.14788100	-1.39540300	-0.64991100
H	-6.22150100	-1.51387700	-0.49441100
C	-0.17039500	3.74477100	-0.68012000
C	1.66647400	1.76856300	-1.37828600
C	-4.47720700	-0.31465300	-0.06553700
C	-3.06676000	-2.17984500	-1.62299900
H	-0.88369000	4.52524700	-0.40500800
H	2.37337100	0.98628900	-1.65148500
H	-5.01012600	0.41363000	0.54762800
H	-2.51081100	-2.90606300	-2.21682600
H	-4.96728400	-3.16442900	-1.87991800
N	-2.40376000	0.94237800	0.33222900
C	-1.83225800	0.85415500	1.56150500
C	-1.86254100	-0.49373900	2.27401000
H	-1.77099600	-1.31386900	1.54919300
H	-2.83905900	-0.62861600	2.76368900
C	-0.77441700	-0.59290300	3.33925100
H	-0.66735000	-1.62644900	3.68607500
H	-0.98319100	0.05838500	4.19517900
H	0.47795000	0.85762400	2.57705400
H	0.83695200	-0.63090500	1.92444800
N	0.55842000	-0.14624900	2.79528200
O	-1.22944400	1.81754900	2.06328600
C	2.98765800	-1.22808500	-0.00847500
C	3.74952600	-2.22274300	-0.64478100
C	3.62101500	-0.12304600	0.58093900
C	5.13974300	-2.10701800	-0.67793300
H	3.25273100	-3.08073100	-1.10139600
C	5.01186800	-0.01194100	0.52822900
H	3.02187100	0.65384500	1.05666200
C	5.77644200	-1.00269700	-0.09718000
H	5.72961600	-2.88571000	-1.16564700
H	5.49789300	0.85313400	0.98321800
H	6.86407000	-0.91701100	-0.13136600
H	1.30738700	-0.27911300	3.47797200

8.2.6 *E-1_{sp}-2P_{sc}-anti-11 (water)*

C	1.65603300	-0.75922000	-1.81086500
C	2.56977600	1.25836400	-0.57989700
C	1.44720200	2.07890500	-0.28225500
C	0.48818500	-1.61475400	-1.36337100

C	-0.56377100	-1.04963000	-0.59125000
H	1.31048000	0.08616300	-2.41899600
H	2.34980500	-1.35750900	-2.41699100
C	-0.45223500	0.34518300	-0.28383200
C	0.16331300	1.42973900	-0.18154500
N	-2.67733600	1.18459300	-0.19751800
N	-2.27658900	2.33235700	0.11692200
N	-1.28518500	2.94666600	0.21244300
C	-0.63094100	-3.77430300	-1.26400500
H	-0.65758100	-4.83146500	-1.53568500
C	-1.64618000	-3.22341700	-0.47329400
H	-2.46806400	-3.84795900	-0.11786900
C	2.92238000	4.01921400	-0.32726800
C	4.01268300	3.20505900	-0.64845100
H	5.00292000	3.63832800	-0.79848800
C	0.43177300	-2.97237900	-1.69012000
C	-1.61156900	-1.87119100	-0.13708200
C	3.82955800	1.82645100	-0.78387200
C	1.65323700	3.46472200	-0.15526600
H	1.24262000	-3.40858800	-2.27719600
H	-2.39373500	-1.44011700	0.48423300
H	4.66723300	1.17676500	-1.04249100
H	0.80488900	4.10523500	0.07583300
H	3.05679400	5.09709500	-0.21984000
N	2.41793600	-0.16410000	-0.67545500
C	3.04626300	-1.01250700	0.17644300
C	3.71551000	-0.44829500	1.42557900
H	3.25561300	0.50111000	1.72675600
H	4.76998800	-0.22742100	1.19275800
C	3.62435800	-1.41674800	2.60357800
H	2.57955200	-1.65127000	2.84216700
H	4.11073900	-1.00088200	3.49277000
H	3.91231900	-2.99265600	1.32953000
H	4.09416100	-3.44779600	2.95573600
H	5.30716600	-2.62627700	2.19156700
N	4.29160000	-2.72173600	2.26459400
O	3.05725600	-2.24138100	-0.03858200
C	-3.97345900	0.74058400	0.16710500
C	-4.65289100	1.22070900	1.29979900
C	-4.55163000	-0.25725600	-0.63234000
C	-5.90993100	0.70443700	1.61813600
H	-4.19532200	1.99517400	1.91837300
C	-5.80275000	-0.77722900	-0.29398200
H	-4.01031100	-0.61839300	-1.50766000
C	-6.48752200	-0.29816600	0.82860500
H	-6.43929900	1.08524300	2.49411300
H	-6.24706800	-1.55579900	-0.91733800
H	-7.46827000	-0.70202200	1.08717900

8.2.7 *E-1_{sp}-2M_{sc}-syn-11 (water)*

C	-2.08046900	2.12291400	-0.53252000
C	-3.10341400	-0.16489300	-0.28306200
C	-2.37115400	-1.10837200	-1.05295900
C	-0.59790400	2.40681700	-0.74419500

C	0.35483900	1.39722700	-1.06075600
H	-2.56020700	1.93902400	-1.50324800
H	-2.55404300	3.01277700	-0.09504000
C	-0.09062300	0.03585200	-1.06434700
C	-0.95484000	-0.86555900	-1.13664400
N	1.57831500	-1.24737800	0.06135100
N	0.95506300	-2.33169700	-0.16214400
N	-0.08680500	-2.68822100	-0.55352700
C	1.15599500	4.08366600	-1.01097800
H	1.46045800	5.13178700	-0.98238100
C	2.08047500	3.08952200	-1.34835400
H	3.11240400	3.35137900	-1.58895200
C	-4.42417100	-2.34179700	-1.43317100
C	-5.13933600	-1.40706400	-0.67612200
H	-6.21447500	-1.52498300	-0.53100400
C	-0.16516100	3.73691300	-0.71240900
C	1.68083500	1.75506200	-1.36820300
C	-4.47649000	-0.31795000	-0.09845000
C	-3.04632300	-2.20126200	-1.61539500
H	-0.88232300	4.51962600	-0.45416700
H	2.39144000	0.97091200	-1.62559200
H	-5.01693700	0.41748900	0.49940600
H	-2.48294600	-2.93447000	-2.19341700
H	-4.94264900	-3.19172000	-1.88079600
N	-2.40893500	0.94588900	0.30735900
C	-1.85520700	0.87398300	1.54568100
C	-1.89939800	-0.46353600	2.27644600
H	-1.79922000	-1.29402100	1.56474000
H	-2.88375400	-0.58898100	2.75275400
C	-0.82889300	-0.54959800	3.36024800
H	-0.73046600	-1.57774500	3.72507700
H	-1.04943100	0.11570900	4.20226900
H	0.43836200	0.88378700	2.58937800
H	0.80926100	-0.61944400	1.97951200
N	0.51414600	-0.11500500	2.83184300
O	-1.25791000	1.84347200	2.04254500
C	2.99656200	-1.22939600	0.01057100
C	3.75299400	-2.21802100	-0.64160000
C	3.63471500	-0.12967000	0.60440000
C	5.14278800	-2.10153300	-0.68650200
H	3.25220900	-3.07163600	-1.10209900
C	5.02499300	-0.01734200	0.53970300
H	3.03894500	0.64153500	1.09333900
C	5.78420200	-1.00197000	-0.10183700
H	5.72849000	-2.87540600	-1.18678700
H	5.51498200	0.84370200	0.99809200
H	6.87142800	-0.91523800	-0.14557800
H	1.24916700	-0.23093800	3.53268400

8.3 Methyl Azide (MeN₃) + Non-Protonated (NH₂) alkyne

8.3.1 *E*-1*M*-2*M*_{sc}-syn-12

C	-1.04011000	-1.45015000	-1.33223700
C	1.36735400	-1.18601600	-0.72859400
C	1.63012600	0.19929200	-0.90001600
C	-2.20924700	-0.58775100	-0.89669500

C	-2.03644700	0.78384200	-0.55597500
H	-0.57665000	-1.01546600	-2.22749900
H	-1.40699000	-2.45207600	-1.59512600
C	-0.69016900	1.29700400	-0.52272900
C	0.53881400	1.09461600	-0.64470600
N	-0.76053600	3.43730200	0.21973200
N	0.39262900	3.53540600	0.34461300
N	1.48698700	2.98652800	0.08036000
C	-4.61511600	-0.34211000	-0.58723000
H	-5.61296200	-0.78549400	-0.59932500
C	-4.44524800	1.00714100	-0.26009700
H	-5.30964800	1.62778700	-0.01528800
C	3.89905800	-0.35080800	-1.59027200
C	3.63344100	-1.71382100	-1.41240900
H	4.40779300	-2.45699200	-1.61077700
C	-3.49989900	-1.12587000	-0.89720700
C	-3.16639100	1.56364300	-0.24081300
C	2.36422800	-2.12780300	-0.99934100
C	2.90547400	0.59627000	-1.34231700
H	-3.63073500	-2.18093900	-1.14743800
H	-3.02885300	2.61114300	0.02091200
H	2.13487700	-3.18806600	-0.87995000
H	3.10074000	1.65661600	-1.50209300
H	4.88326100	-0.02439300	-1.93132800
N	0.05581300	-1.60508800	-0.33907600
C	-0.22532300	-2.29751000	0.81246800
C	0.80881000	-2.34981900	1.92265100
H	1.83332300	-2.19840200	1.56111500
H	0.74381200	-3.35430000	2.36665000
C	0.49458300	-1.29606800	3.01152700
H	1.13989100	-1.50543200	3.87894400
H	-0.54697600	-1.42251700	3.34684300
H	1.64560800	0.24155300	2.29468500
H	0.09481600	0.34267100	1.82890800
N	0.68996900	0.10334500	2.62032900
O	-1.34606400	-2.79550000	0.98174400
C	2.52591400	3.00083800	1.12407400
H	3.28147500	2.26735300	0.81993600
H	3.00366100	3.99009500	1.18716900
H	2.11892800	2.71889100	2.10752300

8.3.2 *E-1M-2M_{sc}-anti-11*

C	0.01593400	-1.08661000	-1.70493400
C	2.00263800	0.06037700	-0.66165300
C	1.52201700	1.33434300	-0.24854500
C	-1.35394600	-1.23562800	-1.07325400
C	-1.85752000	-0.22957500	-0.20259300
H	0.08303200	-0.14326900	-2.26139900
H	0.19521200	-1.91265900	-2.40665400
C	-1.00864400	0.90607000	0.03092600
C	0.11632600	1.45353000	0.02986900
N	-2.39808200	2.61315400	0.55313900
N	-1.47369300	3.45400000	0.61719000
N	-0.31648900	3.58205000	0.62847900
C	-3.39760200	-2.51779700	-0.73652900

H	-3.99519500	-3.40585000	-0.95218700
C	-3.87672800	-1.54287600	0.14600300
H	-4.84783900	-1.66711000	0.62937400
C	3.77618500	2.22604500	-0.51744400
C	4.23218400	0.97715000	-0.95301200
H	5.27746900	0.83712300	-1.23441300
C	-2.14075100	-2.36229500	-1.32874600
C	-3.11287500	-0.40627800	0.41039600
C	3.34152700	-0.09595700	-1.03529800
C	2.43441100	2.40411900	-0.17913100
H	-1.75214400	-3.13584700	-1.99396800
H	-3.47229400	0.35035000	1.10737700
H	3.68126900	-1.07559400	-1.37615500
H	2.07434800	3.38014700	0.14114200
H	4.46603000	3.06953600	-0.45178200
N	1.12108400	-1.06496300	-0.70778200
C	1.34263900	-2.22005000	0.00609900
C	2.24047500	-2.17361500	1.22898200
H	2.91216000	-1.30700000	1.23497500
H	2.85293900	-3.08782500	1.22411900
C	1.36929000	-2.15014000	2.50802400
H	2.03909700	-2.24644300	3.37677300
H	0.70735100	-3.03003000	2.50935300
H	1.12771700	-0.11586100	2.66016300
H	-0.11289400	-0.84898900	1.91773500
N	0.54384400	-0.95089000	2.68970800
O	0.71973100	-3.25336500	-0.26763700
C	-3.58657100	2.96481900	-0.24235300
H	-4.19393700	3.72263800	0.27558500
H	-3.31119300	3.32781300	-1.24481200
H	-4.17956400	2.04854800	-0.34010600

8.4 Methyl Azide (MeN₃) + Protonated (NH₃⁺) alkyne

8.4.1 *E-1_{sp}-2P_{sc}-syn-12*

C	1.01608500	0.55972100	-1.76084100
C	-1.33857000	0.94305500	-0.97728700
C	-1.84684300	-0.35143500	-0.69331800
C	2.05653900	-0.35252100	-1.14090600
C	1.68769100	-1.49980800	-0.38253600
H	0.39455600	-0.00684800	-2.46596500
H	1.51774800	1.36122600	-2.32073600
C	0.28584400	-1.70921200	-0.12195500
C	-0.89951000	-1.32277200	-0.22865300
N	0.07054800	-3.56899300	1.15625800
N	-1.06755200	-3.42290300	1.35192800
N	-2.07744900	-2.77036500	1.00275400
C	4.40407600	-0.95976900	-0.89347900
H	5.45559500	-0.74386300	-1.09344700
C	4.04205200	-2.09107100	-0.15537600
H	4.80897500	-2.76780800	0.22684700
C	-4.04537600	0.40999900	-1.41024500
C	-3.53429200	1.68580800	-1.67383300
H	-4.18638800	2.47449900	-2.05266600
C	3.41188800	-0.10062200	-1.37455700
C	2.69672700	-2.35617600	0.10013200

C	-2.17559500	1.94517900	-1.47149800
C	-3.21076300	-0.60022200	-0.93057900
H	3.69331200	0.78637200	-1.94650500
H	2.41256800	-3.23120200	0.68151200
H	-1.75383200	2.92489000	-1.70216800
H	-3.60310500	-1.60075900	-0.75158400
H	-5.10127600	0.19709900	-1.58692100
N	0.06332900	1.19087900	-0.80634900
C	0.55304900	2.04415100	0.12188800
C	-0.40507400	2.62851600	1.15573900
H	-1.20935200	1.91798900	1.38751700
H	-0.89331500	3.51766500	0.72480300
C	0.30509400	2.98917500	2.45799800
H	0.77991500	2.10785000	2.90640200
H	-0.39262300	3.42743600	3.17976000
H	1.95931900	3.57433300	1.40993400
H	1.99786700	4.12523700	3.01746900
H	1.04243200	4.89207600	1.90781500
N	1.40577300	3.98091100	2.19752700
O	1.76539400	2.34178100	0.14335400
C	-3.00916300	-2.34205500	2.06042200
H	-2.48132800	-1.84871600	2.89139200
H	-3.70221500	-1.63020400	1.59821800
H	-3.58771200	-3.19786000	2.43996900

8.4.2 *E-1_{sp}-2P_{sc}-anti-11*

C	0.28236500	-0.68196000	-1.76231400
C	1.41441900	1.30443800	-0.67468300
C	0.36226000	2.09185500	-0.13233600
C	-0.76986300	-1.56529700	-1.12325200
C	-1.66421300	-1.03833200	-0.15110500
H	-0.18176900	0.18074300	-2.25646900
H	0.84087900	-1.25053300	-2.51856900
C	-1.51752300	0.35167900	0.18105100
C	-0.86191200	1.41725600	0.20513400
N	-3.54693700	1.01845500	0.95061100
N	-3.19188800	2.21042800	1.08498800
N	-2.26998700	2.92254500	1.06628400
C	-1.83500200	-3.74388200	-0.89716200
H	-1.90279600	-4.79171400	-1.19641400
C	-2.69075300	-3.23341200	0.08553000
H	-3.42602200	-3.88179400	0.56615500
C	1.76926700	4.06356000	-0.40986900
C	2.78560000	3.28081000	-0.96712800
H	3.71909900	3.73902300	-1.29812500
C	-0.87686300	-2.91181800	-1.48301300
C	-2.60558600	-1.89176900	0.45559900
C	2.60003100	1.90289400	-1.10777200
C	0.56865100	3.47816000	-0.00552400
H	-0.18775000	-3.31575600	-2.22760100
H	-3.25591100	-1.49325100	1.23341500
H	3.37857500	1.27946300	-1.55071000
H	-0.22823000	4.09199700	0.41003100
H	1.90729800	5.14066100	-0.29847200
N	1.25929400	-0.11669300	-0.78748200

C	2.04822500	-0.98186300	-0.10487200
C	2.95139000	-0.44034800	0.99928500
H	2.51947900	0.46156000	1.45184900
H	3.91371700	-0.13673000	0.55685500
C	3.17679600	-1.46749500	2.10602400
H	2.22637000	-1.77782300	2.55712000
H	3.83076400	-1.06604900	2.88765300
H	3.22689700	-2.97227300	0.72319500
H	3.83268200	-3.47286800	2.22985800
H	4.77020200	-2.54666100	1.23213700
N	3.81176300	-2.71196500	1.54842400
O	2.02523500	-2.20465700	-0.35325600
C	-4.83149500	0.76046800	0.27767800
H	-5.67547400	1.03858200	0.92725800
H	-4.90382200	1.29956600	-0.67972400
H	-4.87654800	-0.31794600	0.08919100

9 Characterization of Interaction of Individual Reactants with SDS by Investigating the Effect on Effective Mobility

Dependence of mobility of all substrates on concentration of SDS was measured at acidic pH (15mM citric acid / 10 mM LiOH, 0–50 mM SDS) and basic pH (7 mM β -AL / 10 mM LiOH, 0–50 mM SDS). The measurements at acidic pH were performed using the PreMCE method to be able to precisely determine the anionic mobilities using an uncoated capillary. The method was performed in the following setup: injection of analyte at 50 mbar for 5 s, plug of buffer at 50 mbar for 2 min, EOF marker injected at 50 mbar for 5 s, voltage applied: 20 kV. In the case of Ph-AL-AZ, the dependence was observed also in maleic acid buffer (13 mM maleic acid / 5.5 mM Li), mobilities were measured by short end injection. Concentration of observed analytes was always 1 mM.

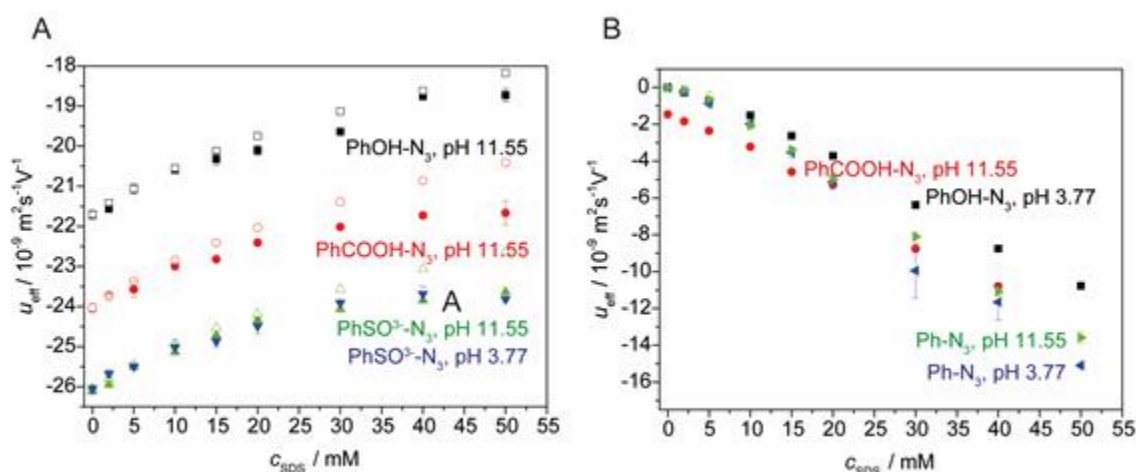


Figure SI-7 The dependence of effective mobility of the reactants on the concentration of SDS in the BGE. A) Charged azides; solid symbols represent experimental data, transparent symbols represent the mobilities predicted theoretically by PeakMaster 5.3; mobilities corrected for increasing ionic strength: black squares AZ-OH, pH 11.55 (at SDS 0 mM), red circles AZ-COOH, pH 11.55 (at SDS 0 mM), green upward triangles AZ-SO₃⁻, pH 11.55 (at SDS 0 mM), blue downward triangles AZ-SO₃⁻, pH 3.77. B) Neutral azides: black squares AZ-OH, pH 3.77 (at SDS 0 mM), red circles AZ-COOH, pH 3.77 (at SDS 0 mM), green rightward triangles AZ, pH 11.55 (at SDS 0 mM), blue leftward triangles AZ, pH 3.77 (at SDS 0 mM).

10 Determination of the Critical Micelle Concentration (CMC)

10.1 FCS Measurements

Rhodamine 123 was used as dye for determination of the critical micelle concentration (CMC) by fluorescent correlation spectroscopy (FCS). The concentration of Rhodamine 123 in each sample was 10 nM with 20mM MOPS / 10mM LiOH buffer (pH 7.16, IS 10 mM) as running buffer. The content of MeCN in the running buffer was 28 vol%. FCS measurements were performed at various concentrations of SDS in the range of 0 mM to 100 mM SDS. The measurements were performed in triplicates. Autocorrelation curves were fitted by suitable theoretical functions. According to literature, the obtained autocorrelation function can be fitted by either one componential or two componential fitting models. In a first step, the data was evaluated by one componential fitting and the diffusion coefficient was determined. The diffusion time of free dye (SDS free solution) obtained by the one componential fit was used as fixed input parameter for the two componential fitting. We were then able to determine the diffusion coefficient of the interacted dye as well as the fraction of the interacting and free form of the dye. The CMC was determined from the inflection point of the dependence of the diffusion coefficient (obtained by one component fitting) and the fraction of complexed dye (obtained by two componential fit on the concentration of SDS). The resulting dependences are shown in Figure SI-7.

10.2 Mobility Measurements

20 mM MOPS / 10mM LiOH buffer (pH 7.16, IS 10 mM) was used as running buffer, the content of MeCN was 28 vol%. The concentration of SDS in all separation buffers of different MeCN content was varied from 0 mM to 50 mM. Naphthalene and rhodamine 123 in a concentration of 0.5 mM served as suitable probes for mobility measurements, 0.2 vol% DMSO was used as EOF marker. The detection was performed at $\lambda = 214$ nm. The measurements were performed in triplicates. The CMC was calculated by determination of the inflection point of the function showing the dependence of the effective mobility of naphthalene/rhodamine on the concentration of SDS.

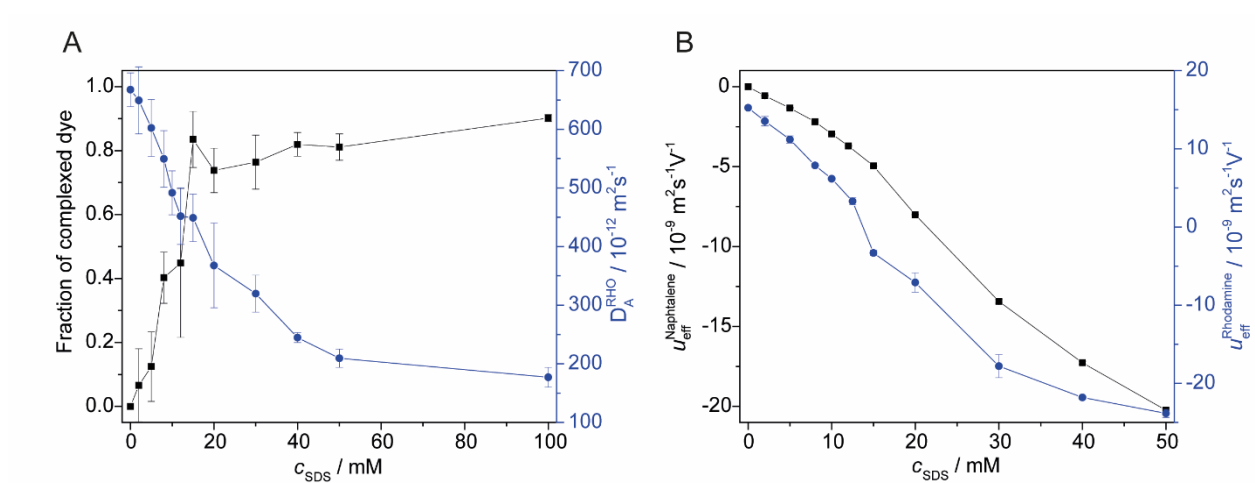
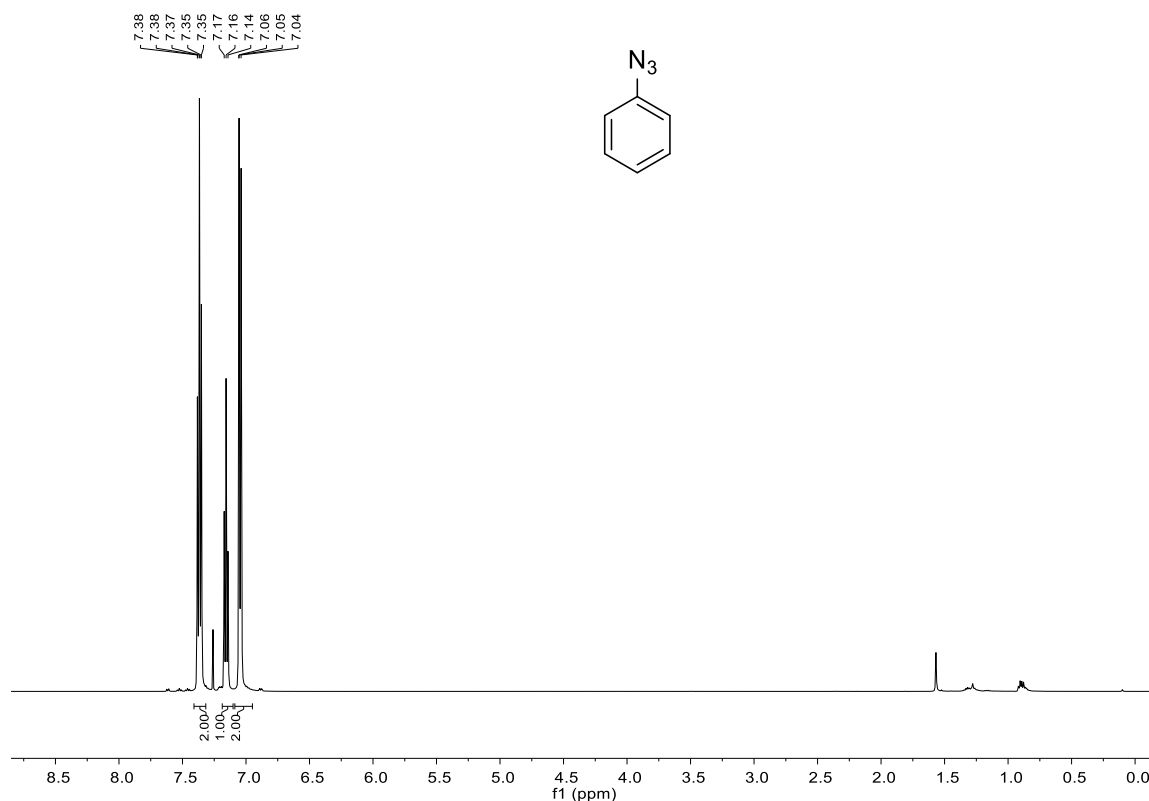


Figure SI-8 A) Dependence of the fraction of complexed rhodamine 123 (black squares, left axes) and diffusion coefficient of rhodamine 123 (blue circles, right axes) on the concentration of SDS. B) Dependence of mobility of naphthalene (black squares, left axes) and rhodamine 123 (blue circles, right axes) on the concentration of SDS.

11 NMR Spectra

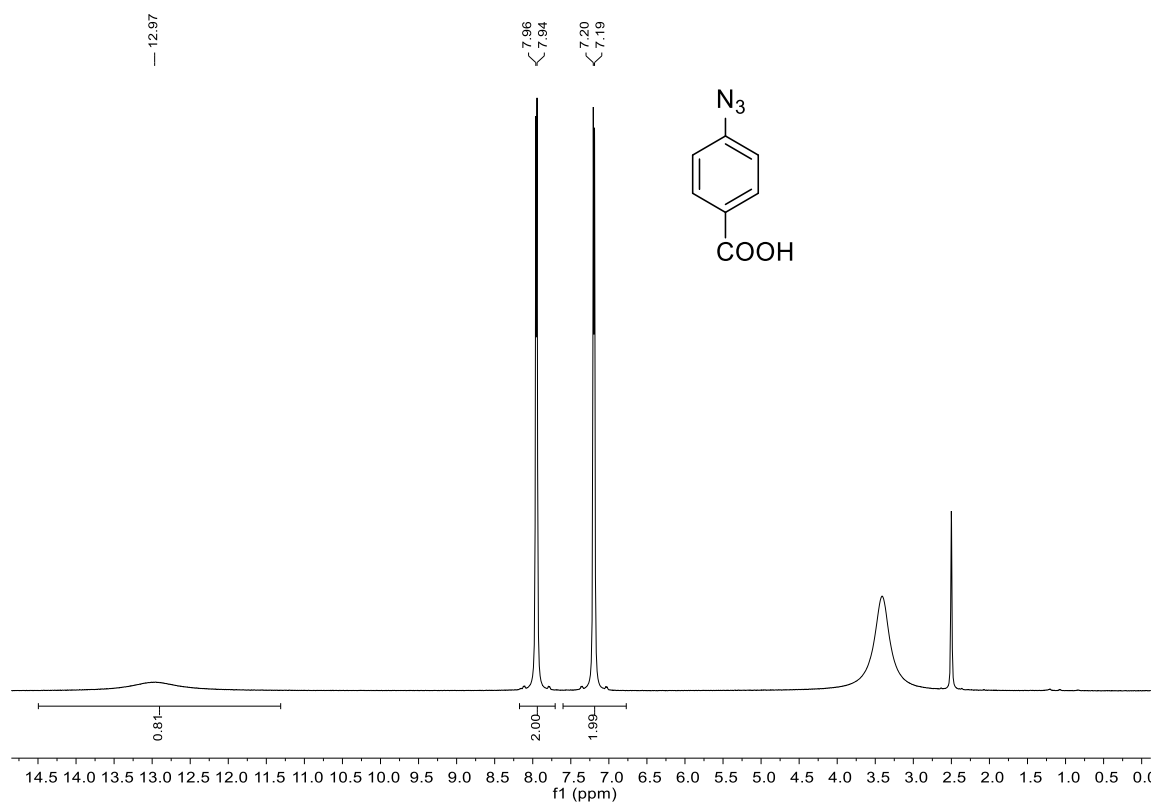
Nuclear magnetic resonance spectra (NMR): ^1H NMR spectra were recorded in CDCl_3 , CD_2Cl_2 , or $\text{DMSO}-d_6$ on the instruments *AV-500* (500 MHz) or *AV-400* (400 MHz); chemical shift δ in ppm relative to solvent signals ($\delta = 7.26$ ppm for CDCl_3 , 5.32 ppm for CD_2Cl_2 , and 2.50 for $\text{DMSO}-d_6$),⁸ coupling constant J is given in Hz. ^{13}C NMR spectra were recorded in CDCl_3 , CD_2Cl_2 , or $\text{DMSO}-d_6$ on the instruments *Bruker AV-500* (125 MHz) or *AV-400* (100 MHz); chemical shift δ in ppm relative to solvent signals ($\delta = 77.16$ ppm for CDCl_3 , 53.84 ppm for CD_2Cl_2 , and 39.52 for $\text{DMSO}-d_6$).⁸

11.1 Phenyl Azide

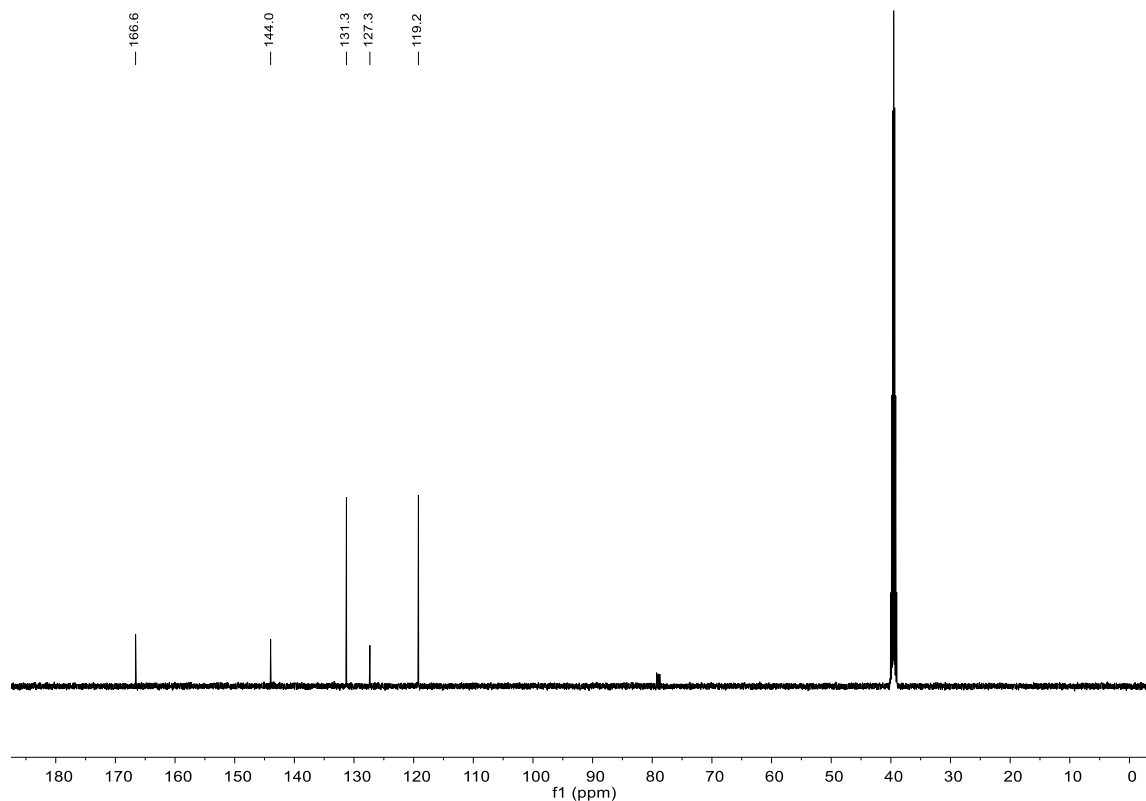


^1H NMR, CDCl_3 , 500.13 MHz, 295.0 K.

11.2 *p*-Azidobenzoic Acid

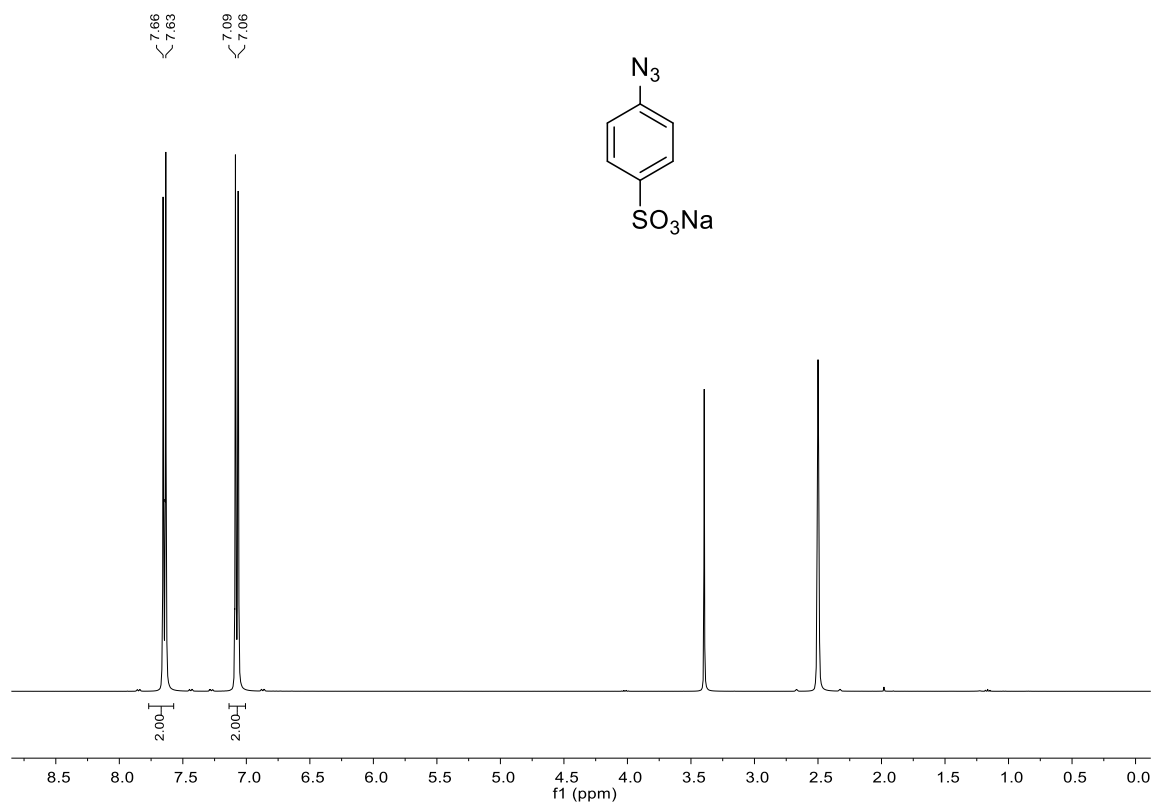


¹H NMR, d₆-DMSO, 500.13 MHz, 295.0 K.

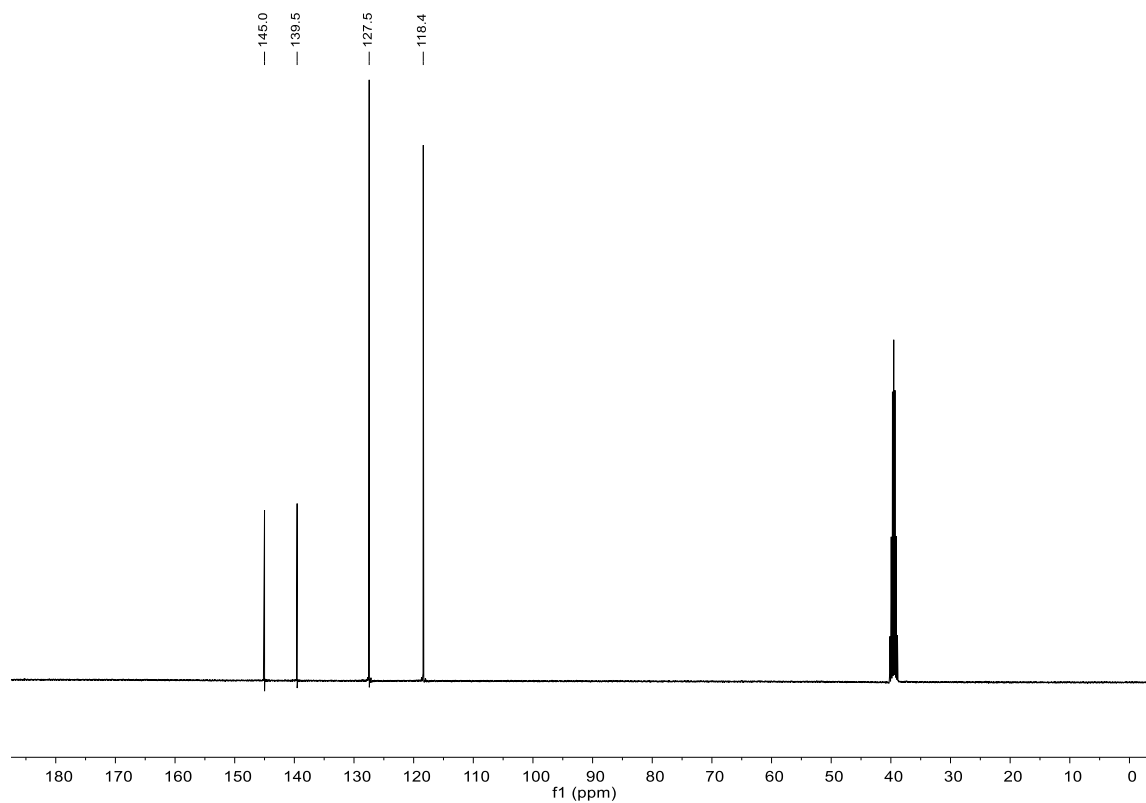


¹³C NMR, d₆-DMSO, 125.77 MHz, 295.1 K.

11.3 Sodium *p*-Azidobenzenesulfonate

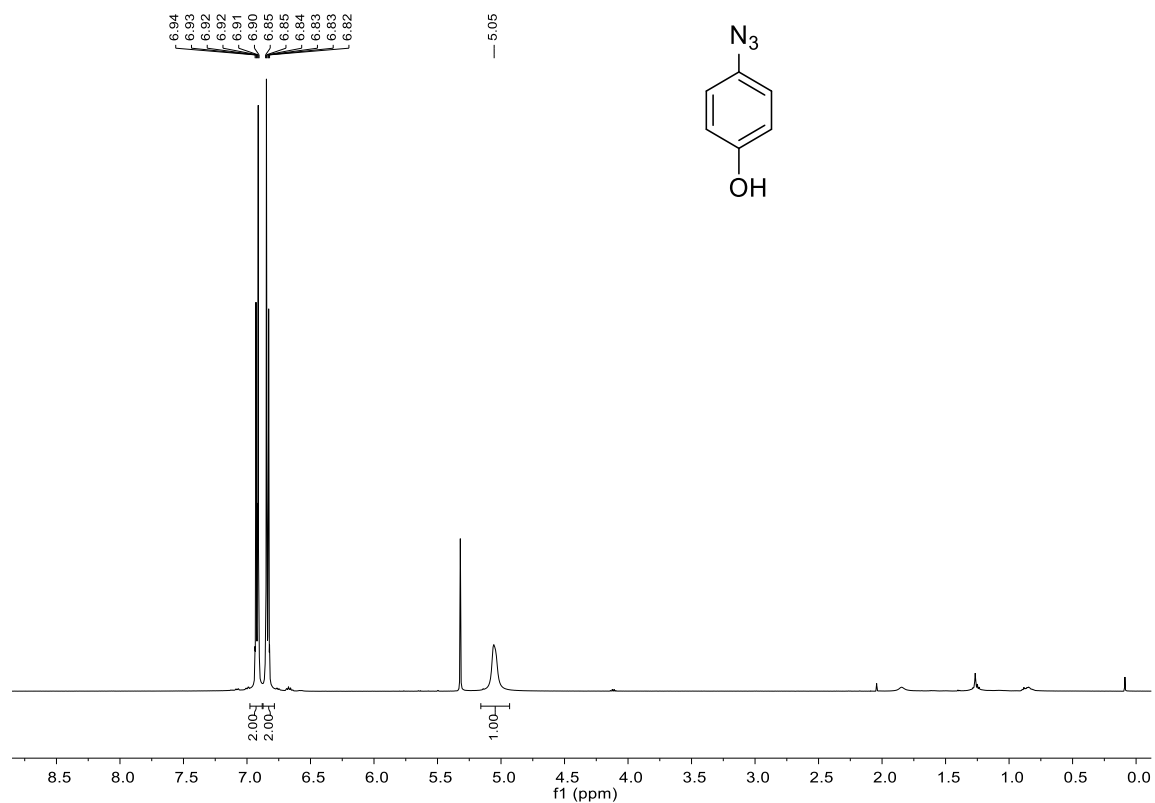


¹H NMR, d₆-DMSO, 400.13 MHz, 295.0 K.

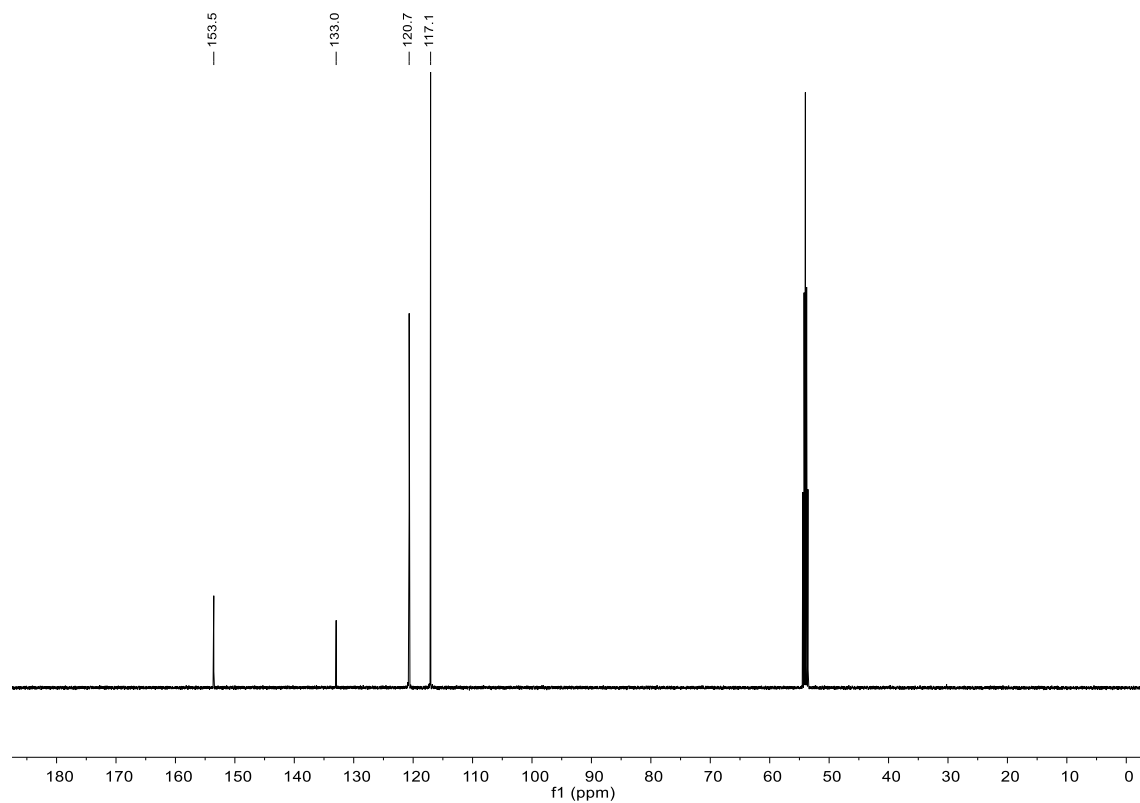


¹³C NMR, d₆-DMSO, 100.62 MHz, 295.0 K.

11.4 *p*-Azidophenol



¹H NMR, CD₂Cl₂, 500.13 MHz, 295.0 K.



¹³C NMR, CD₂C₂, 125.77 MHz, 295.1 K.

12 References

- (1) Nguyen, D. M.; Miles, D. H. *Synth. Commun.* **2011**, *41*, 1759.
- (2) Ryu, B.-Y.; Emrick, T. *Macromolecules* **2011**, *44*, 5693.
- (3) Hradilová, L.; Poláková, M.; Dvořáková, B.; Hajdúch, M.; Petruš, L. *Carbohydr. Res.* **2012**, *361*, 1.
- (4) Nonogaki, S.; Toriumi, M. *J. Macromol. Sci. A* **1988**, *25*, 617.
- (5) Davis, D. L.; Price, E. K.; Aderibigbe, S. O.; Larkin, M. X. H.; Barlow, E. D.; Chen, R.; Ford, L. C.; Gray, Z. T.; Gren, S. H.; Jin, Y.; Keddington, K. S.; Kent, A. D.; Kim, D.; Lewis, A.; Marrouche, R. S.; O'Dair, M. K.; Powell, D. R.; Scadden, M. I. H. C.; Session, C. B.; Tao, J.; Trieu, J.; Whiteford, K. N.; Yuan, Z.; Yun, G.; Zhu, J.; Heemstra, J. M. *J. Org. Chem.* **2016**, *81*, 6816.
- (6) Debets, M. F.; van Berkel, S. S.; Schoffelen, S.; Rutjes, F. P. J. T.; van Hest, J. C. M.; van Delft, F. L. *Chem. Commun.* **2010**, *46*, 97.
- (7) Dommerholt, J.; Rutjes, F. P. J. T.; van Delft, F. L. *Top. Curr. Chem.* **2016**, *374*, 16.
- (8) Fulmer, G. R.; Miller, A. J. M.; Sherden, N. H.; Gottlieb, H. E.; Nudelman, A.; Stoltz, B. M.; Bercaw, J. E.; Goldberg, K. I. *Organometallics* **2010**, *29*, 2176.