

Supporting Information

Kinetics of Electrophilic Alkylations of Barbiturate and Thiobarbiturate Anions

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For the reaction of electrophile **4a** with **MB**, the structure of the corresponding acid $\text{N-E}^{\ominus} \text{H}^+$ relates to that of $\text{H}^{\ominus} \text{N-E}$ as well as $\text{H}^+ \text{N}^{\ominus}$. However, the pK_a of $\text{N-E}^{\ominus} \text{H}^+$ should be smaller than that of $\text{E}^{\ominus} \text{H}^+$. For instance, the phenyl substitution increases the acid strength of 2-phenyl barbituric acid ($\text{pK}_a = 2.54$ in water)^[1] compared to barbituric acid ($\text{pK}_a = 3.9$ in water).^[2] That modification would have consequence on actual K -values (Scheme 10). K is estimated to be in the range between 100 or 1000 Lmol^{-1} for the **4a/MB** system. Accordingly, an incomplete conversion of **4a** with **MB** is experimentally found (see Figure 2, left part, as example). The equilibrium constants for 1:1 stoichiometry have been determined for those combinations which show incomplete conversion taking into account the concentration of the electrophile which is measured after reaching the equilibrium state after about one second (for example see Figure 2, left part). Results of the equilibrium measurements for electrophile **4a** are compiled in Table S1. The magnitude of the equilibrium constant for each combination is confirmed by independently determined K -values which are derived from the k_2/k_{-1} ratio. k_{-1} can be estimated from ordinate intercept according to Figure 2, right part. The agreement of both K -values for the **4a/MB** system is coherent. For the **4a/ESB** it is not possible to calculate reasonable K values if assuming the 1:1 equilibrium from the concentration measurements due to K is a function of **ESB** concentration (see Table S1). Using constant anion, for electrophile **3a** the K -values are significantly greater than for **4a** which is expected. The equilibrium constants calculation also shows that the consideration above, K is about 10^2 to 10^3 Lmol^{-1} for the **4a/MB** system, has been confirmed. Thus, the equilibrium constants K of the $\text{E} + \text{N}^{\ominus}$ combinations can be speculatively estimated by $\text{pK} \approx \Delta\text{pK}_a + 3$, if ΔpK_a is simply obtained from the pK_a -values of the corresponding acids of the reactants (see discussion of Table 3). The number 3 comes from the pK_a -difference of barbituric acid derivatives and 2-phenylbarbituric acid which is used to adapt the molecular structure change after the C-C-bond formation reaction.

From the incomplete conversion, the equilibrium constants ($K_{\text{conversion}}$) and the rate constants of the back reaction ($k_{-1, \text{conversion}}$) were calculated and compared with rate constants determined by the axis interception ($k_{-1, \text{kinetic}}$) and the thereby calculated equilibrium constant (K_{kinetic}) (Table S1).

Indeed, the k_{PT}/k_{-1} -value for electrophile **6** type/barbiturate combinations is always less than 1 (Table 4). But the values are not that small as found for electrophile **5**, which means that the extreme scenario considered according to eq. 4 is not completely accomplished for these nucleophile/electrophile combination. For instance, the faster the C–C-bond formation occurs for the electrophiles of type **6**, the faster also the proton transfer reaction takes place as indicated by the k_{PT}/k_{-1} ratio. The deviation of $k_{2,\text{calculated}}$ in relation to $k_{2,\text{obs}}$ increases steadily with increasing $\Delta G^\ddagger$ (theoretically calculated). In the same way the rate constant for the proton transfer should decrease significantly. Therefore, two interfering effects, a low concentration of $^{\ominus}\text{N-E}$ and a depressed proton transfer rate, may be responsible for the deviating kinetics. The subsequent proton transfer step should take place very fast for the electrophiles of type **6** if the C–C-bond formation is irreversible

Table S1 Equilibrium constant (K) calculated by the incomplete conversion of nucleophile-electrophile reactions (left columns) and from the axis interception of the plots $k_{2,\text{obs}}/[\text{N}^{\ominus}]$ (right column).

N/E-combination	conversion	$K_{\text{conversion}}$ [Lmol ⁻¹]	$k_{-1,\text{conversion}}$ [s ⁻¹]	$k_{-1,\text{kinetic}}$ [s ⁻¹]	K_{kinetic} [Lmol ⁻¹]
MB / 4a	0.285	424	5.99	5.34	475
MB / 4a	0.42	460	5.52		
MB / 4a	0.503	458	5.54		
MB / 4a	0.566	459	5.54		
MB / 4a	0.625	479	5.30		
B / 4a	0.508	3389	3.10×10^{-2}	1.40×10^{-2}	7292
B / 4a	0.594	3323	3.16×10^{-2}		
B / 4a	0.679	3396	3.09×10^{-2}		
B / 4a	0.758	3488	3.01×10^{-2}		
ESB / 4a	0.325	1196	3.75×10^{-2}	4.80×10^{-2}	935
ESB / 4a	0.537	1431	3.13×10^{-2}		
ESB / 4a	0.689	1811	2.47×10^{-2}		
ESB / 4a	0.796	2394	1.87×10^{-2}		
ESB / 4a	0.861	3026	1.48×10^{-2}		
SB / 4a	0.945	37809	4.84×10^{-4}	1.00×10^{-4}	182000
SB / 4a	0.97	49715	3.66×10^{-4}		

Kinetic experiments

General Procedure:

All reactions were performed in dry DMSO (< 0.005% water) from Acros Organics at 20 °C. Fast reactions ($\tau_{1/2} < 100$ s) were measured at stopped-flow spectrophotometer system Hi-Tech SF-61DX2, for slower reactions a UV/vis spectrometer MCS 400 from the Carl Zeiss Jena GmbH with optical immersion probe were used. The rate constants k_{obs} (s⁻¹) were obtained by fitting the function $A_t = A_0 \cdot \exp(-k_{\text{obs}} \cdot t) + C$ at the plot of the electrophil absorption over the time. The barbiturate anions were used as potassium salts.

The given errors were determined by RGP-function with Microsoft Excel 2013. The maximal error of $\log k_2$ is ± 0.02 .

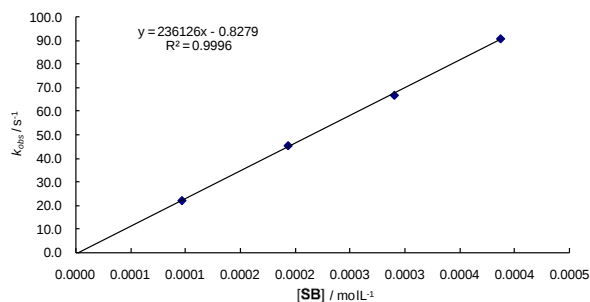
cationic electrophiles

reactions of 1c

reactions of **1c** with **SB**

DMSO, 20 °C, stopped flow, 620 nm

[SB] / M	$k_{\text{obs}} / \text{s}^{-1}$
9.68E-05	21.96
1.94E-04	45.38
2.90E-04	66.87
3.87E-04	90.97



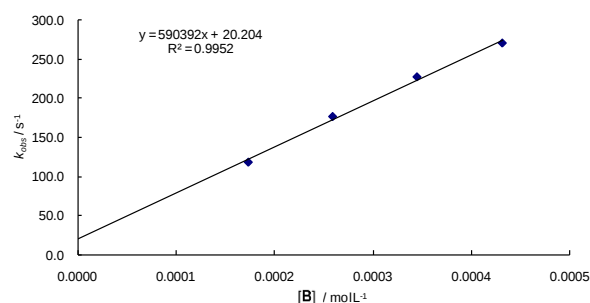
$$k_2 = 236126 \pm 3172.2; C = -0.8279 \pm 0.8406; \log k_2 = 5.37$$

reactions of 1d

reactions of **1d** with **B**

DMSO, 20 °C, stopped flow, 618 nm

[B] / M	$k_{\text{obs}} / \text{s}^{-1}$
1.73E-04	118.40
2.59E-04	177.00
3.45E-04	227.90
4.32E-04	271.30

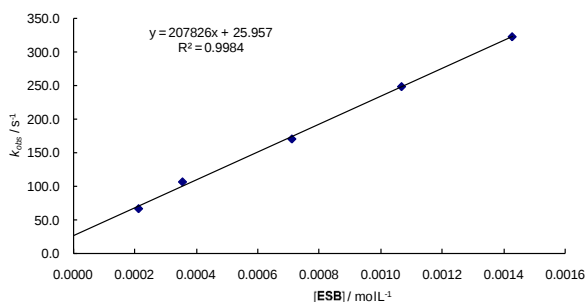


$$k_2 = 590392 \pm 28931; C = 20.204 \pm 9.179; \log k_2 = 5.77$$

reactions of **1d** with **ESB**

DMSO, 20 °C, stopped flow, 618 nm

[ESB] / M	$k_{\text{obs}} / \text{s}^{-1}$
2.14E-04	66.60
3.57E-04	106.60
7.13E-04	170.70
1.07E-03	248.90
1.43E-03	323.40

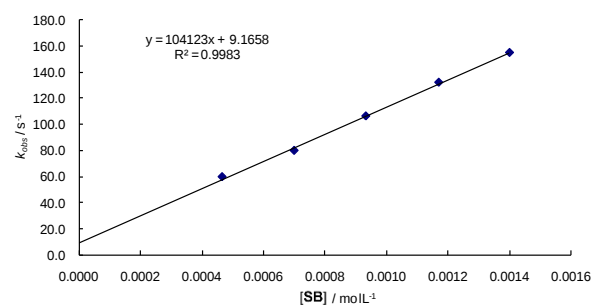


$$k_2 = 207826 \pm 5423.7; C = 25.957 \pm 4.766; \log k_2 = 5.32$$

reactions of **1d** with **SB**

DMSO, 20 °C, stopped flow, 618 nm

[SB] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.66E-04	59.39
7.00E-04	79.59
9.33E-04	106.10
1.17E-03	132.00
1.40E-03	154.90



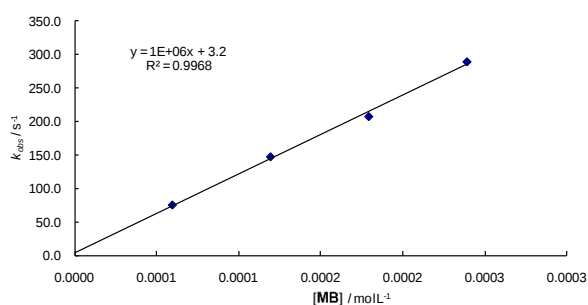
$$k_2 = 104123 \pm 2803.1; C = 9.1658 \pm 2.773; \log k_2 = 5.02$$

reactions of **1e**

reactions of **1e** with **MB**

DMSO, 20 °C, stopped flow, 627 nm

[MB] / M	$k_{\text{obs}} / \text{s}^{-1}$
5.99E-05	74.60
1.20E-04	147.10
1.80E-04	207.60
2.40E-04	289.90

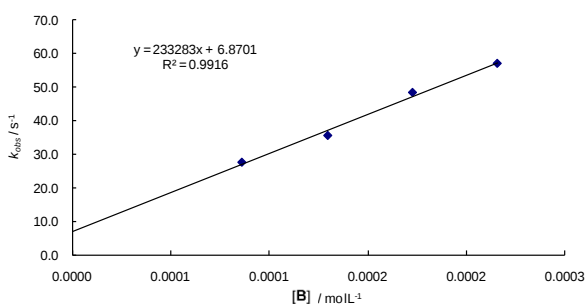


$$k_2 = 1176740 \pm 47503; C = 3.218 \pm 7.805; \log k_2 = 6.06$$

reactions of **1e** with **B**

DMSO, 20 °C, stopped flow, 627 nm

[B] / M	$k_{\text{obs}} / \text{s}^{-1}$
8.64E-05	27.68
1.30E-04	35.63
1.73E-04	48.39
2.16E-04	57.01

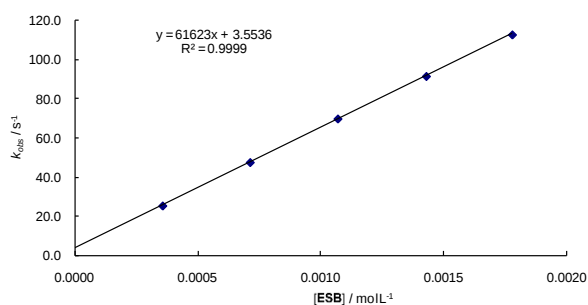


$$k_2 = 233283 \pm 15178; C = 6.8701 \pm 2.411; \log k_2 = 5.37$$

reactions of **1e** with **ESB**

DMSO, 20 °C, stopped flow, 627 nm

[ESB] / M	$k_{\text{obs}} / \text{s}^{-1}$
3.57E-04	25.29
7.13E-04	47.56
1.07E-03	69.90
1.43E-03	91.70
1.78E-03	113.00

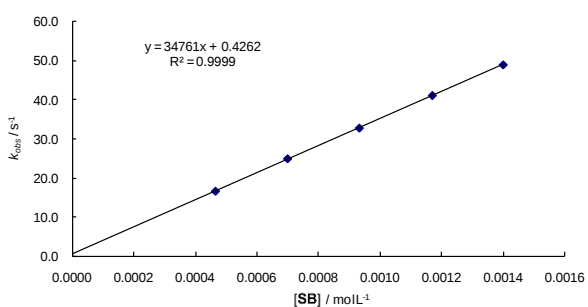


$$k_2 = 61623 \pm 264.58; C = 3.5536 \pm 0.3129; \log k_2 = 4.79$$

reactions of **1e** with **SB**

DMSO, 20 °C, stopped flow, 627 nm

[SB] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.66E-04	16.55
7.00E-04	24.89
9.33E-04	32.78
1.17E-03	41.16
1.40E-03	49.05



$$k_2 = 34761 \pm 254.64; C = 0.4262 \pm 0.2519; \log k_2 = 4.54$$

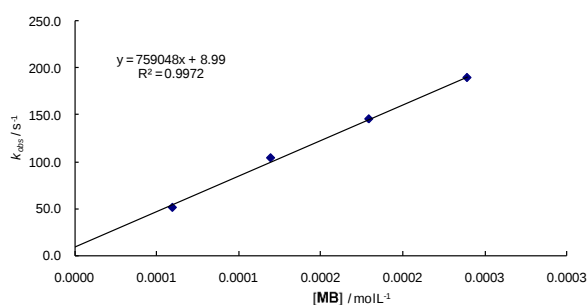
reactions of **1f**

reactions of **1f** with **MB**

DMSO, 20 °C, stopped flow, 635 nm

[MB] / M	$k_{\text{obs}} / \text{s}^{-1}$
5.99E-05	51.58
1.20E-04	104.19
1.80E-04	145.49
2.40E-04	189.37

$$k_2 = 759048 \pm 28007; C = 8.99 \pm 4.602; \log k_2 = 5.88$$

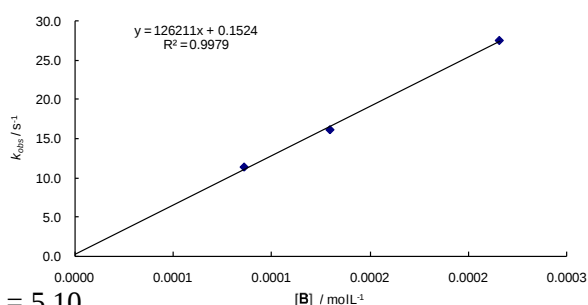


reactions of **1f** with **B**

DMSO, 20 °C, stopped flow, 635 nm

[B] / M	$k_{\text{obs}} / \text{s}^{-1}$
8.64E-05	11.35
1.30E-04	16.13
2.16E-04	27.56

$$k_2 = 126211 \pm 5792.8; C = 0.1524 \pm 0.8913; \log k_2 = 5.10$$

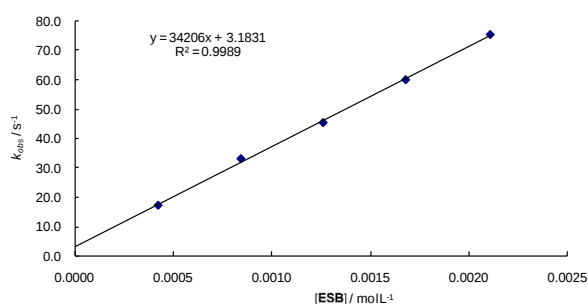


reactions of **1f** with **ESB**

DMSO, 20 °C, stopped flow, 635 nm

[ESB] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.21E-04	17.19
8.42E-04	33.15
1.26E-03	45.54
1.68E-03	60.23
2.11E-03	75.75

$$k_2 = 34206 \pm 731.68; C = 3.1831 \pm 1.022; \log k_2 = 4.53$$

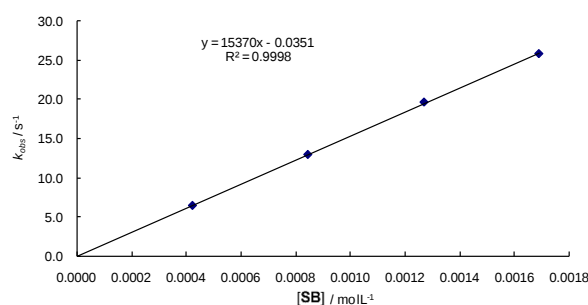


reactions of **1f** with **SB**

DMSO, 20 °C, stopped flow, 635 nm

[SB] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.23E-04	6.42
8.45E-04	12.94
1.27E-03	19.64
1.69E-03	25.84

$$k_2 = 15370 \pm 165.20; C = -0.0351 \pm 0.1912; \log k_2 = 4.19$$

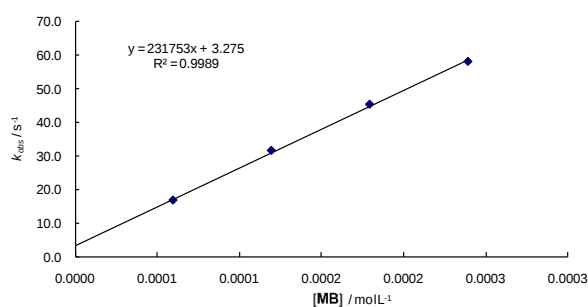


reactions of **1g**

reactions of **1g** with **MB**

DMSO, 20 °C, stopped flow, 630 nm

[MB] / M	$k_{\text{obs}} / \text{s}^{-1}$
5.99E-05	16.64
1.20E-04	31.56
1.80E-04	45.43
2.40E-04	58.29

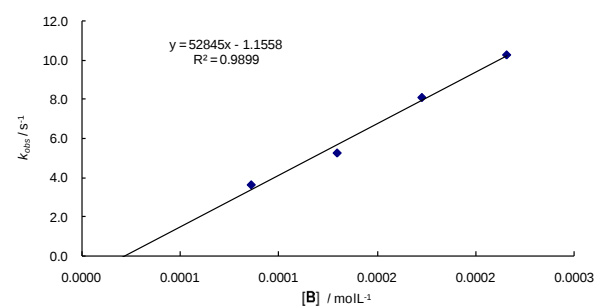


$$k_2 = 231753 \pm 5365.0; C = 3.275 \pm 0.8815; \log k_2 = 5.37$$

reactions of **1g** with **B**

DMSO, 20 °C, stopped flow, 630 nm

[B] / M	$k_{\text{obs}} / \text{s}^{-1}$
8.64E-05	3.65
1.30E-04	5.28
1.73E-04	8.13
2.16E-04	10.31

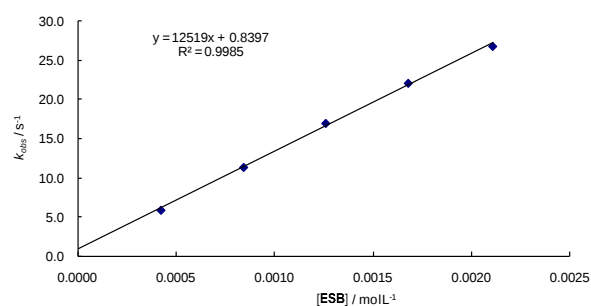


$$k_2 = 52845 \pm 3800.0; C = -1.1558 \pm 0.6037; \log k_2 = 4.72$$

reactions of **1g** with **ESB**

DMSO, 20 °C, stopped flow, 630 nm

[ESB] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.21E-04	5.86
8.42E-04	11.36
1.26E-03	17.00
1.68E-03	22.14
2.11E-03	26.87

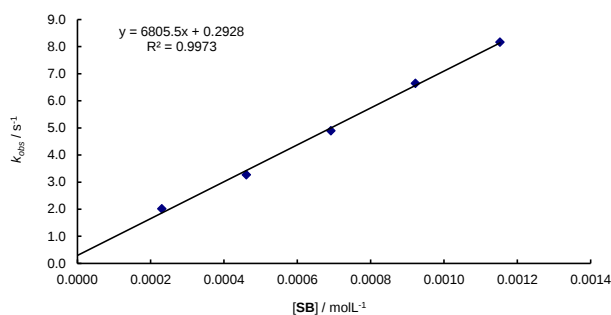


$$k_2 = 12519 \pm 249.57; C = 0.8397 \pm 0.3487; \log k_2 = 4.10$$

reactions of **1g** with **SB**

DMSO, 20 °C, stopped flow, 630 nm

[SB] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.21E-04	2.01
8.2E-04	3.27
1.26E-03	4.89
1.68E-03	6.65
2.11E-03	8.17



$$k_2 = 6805.5 \pm 203.80; C = 0.2928 \pm 0.1558; \log k_2 = 3.83$$

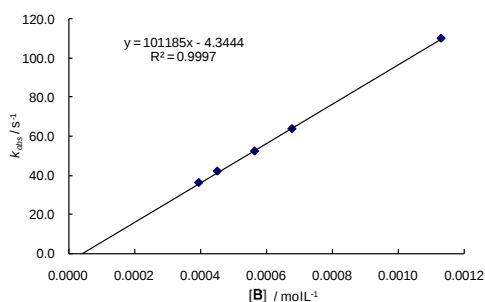
neutral electrophiles

reactions of 2a

reactions of 2a with B

DMSO, 20 °C, stopped flow, 325 nm

[B] / M	$k_{\text{obs}} / \text{s}^{-1}$
3.96E-04	36.031
4.53E-04	41.959
5.66E-04	52.291
6.79E-04	63.810
1.13E-03	110.428

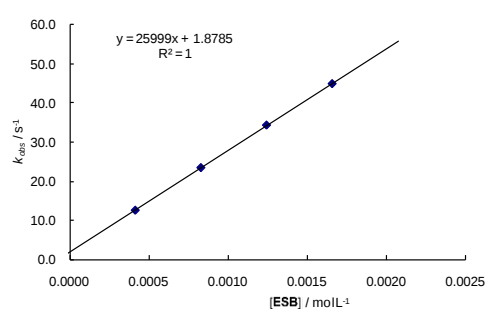


$$k_2 = 101185 \pm 1030.0; C = -4.3444 \pm 0.7169; \log k_2 = 5.01$$

reactions of 2a with ESB

DMSO, 20 °C, stopped flow, 325 nm

[ESB] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.15E-04	12.616
8.31E-04	23.513
1.25E-03	34.387
1.66E-03	44.988

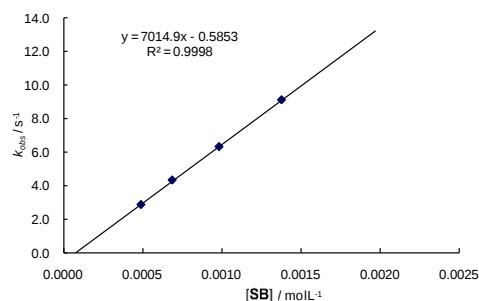


$$k_2 = 25999 \pm 120.45; C = 1.8785 \pm 0.1370; \log k_2 = 4.41$$

reactions of 2a with SB

DMSO, 20 °C, stopped flow, 325 nm

[SB] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.94E-04	2.849
6.91E-04	4.319
9.88E-04	6.316
1.38E-03	9.118



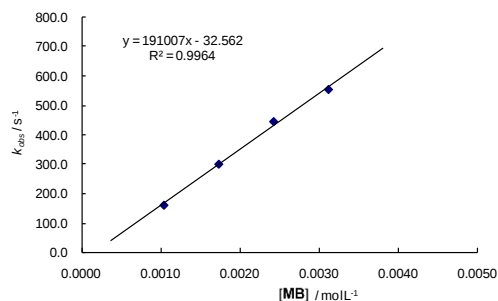
$$k_2 = 7014.9 \pm 71.61; C = -0.5853 \pm 0.068; \log k_2 = 3.85$$

reactions of 2b double designated

reactions of 2b with MB

DMSO, 20 °C, stopped flow, 366 nm

[MB] / M	$k_{\text{obs}} / \text{s}^{-1}$
1.04E-03	160.730
1.74E-03	300.270
2.43E-03	445.220
3.12E-03	554.290

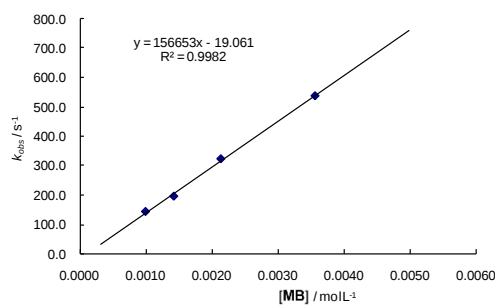


$$k_2 = 191007 \pm 8117; C = -32.560 \pm 18.04; \log k_2 = 5.28$$

reactions of **2b** with **MB**

DMSO, 20 °C, stopped flow, 366 nm

[MB] / M	$k_{\text{obs}} / \text{s}^{-1}$
9.96E-04	141.706
1.42E-03	194.020
2.14E-03	321.942
3.56E-03	537.222

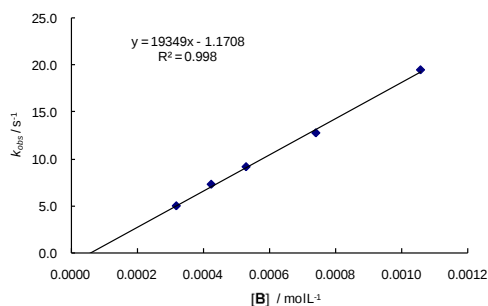


$$k_2 = 156653 \pm 4653; C = -19.061 \pm 10.47; \log k_2 = 5.19$$

reactions of **2b** with **B**

DMSO, 20 °C, stopped flow, 366 nm

[B] / M	$k_{\text{obs}} / \text{s}^{-1}$
3.18E-04	4.933
4.24E-04	7.245
5.30E-04	9.125
7.41E-04	12.755
1.06E-03	19.515

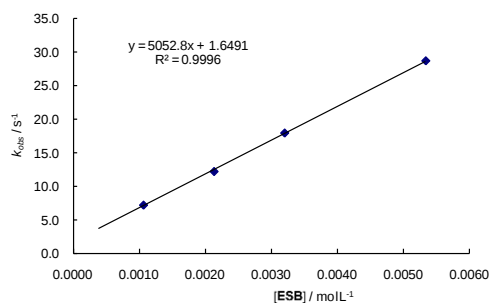


$$k_2 = 19349 \pm 505.8; C = -1.1708 \pm 0.3379; \log k_2 = 4.29$$

reactions of **2b** with **ESB**

DMSO, 20 °C, stopped flow, 366 nm

[ESB] / M	$k_{\text{obs}} / \text{s}^{-1}$
1.07E-03	7.198
2.14E-03	12.200
3.21E-03	17.929
5.34E-03	28.675

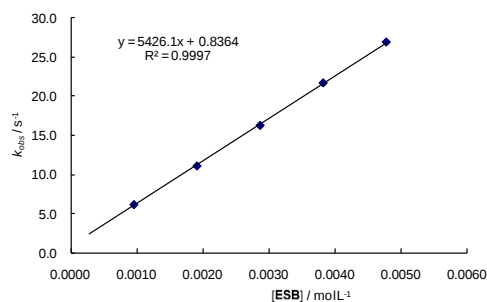


$$k_2 = 5052.8 \pm 67.57; C = 1.6491 \pm 0.2255; \log k_2 = 3.70$$

reactions of **2b** with **ESB**

DMSO, 20 °C, stopped flow, 366 nm

[ESB] / M	$k_{\text{obs}} / \text{s}^{-1}$
9.58E-04	6.187
1.92E-03	11.109
2.87E-03	16.266
3.83E-03	21.681
4.79E-03	26.882

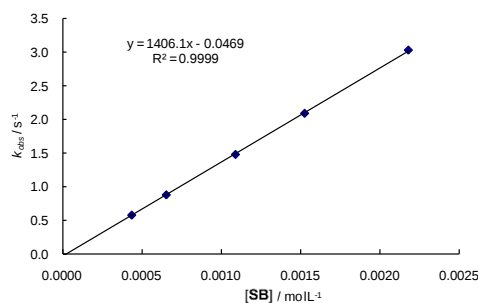


$$k_2 = 5426.1 \pm 50.88; C = 0.8364 \pm 0.1616; \log k_2 = 3.73$$

reactions of **2b** with **SB**

DMSO, 20 °C, stopped flow, 366 nm

[SB] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.37E-04	0.575
6.55E-04	0.877
1.09E-03	1.479
1.53E-03	2.092
2.18E-03	3.034

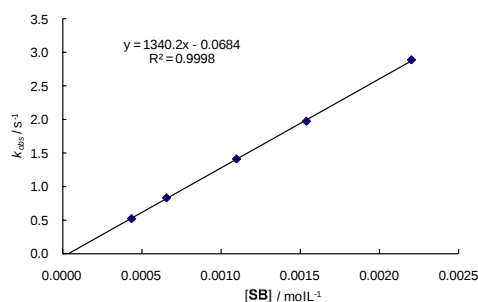


$$k_2 = 1406.1 \pm 7.953; C = -0.0469 \pm 0.011; \log k_2 = 3.15$$

reactions of **2b** with **SB**

DMSO, 20 °C, stopped flow, 366 nm

[SB] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.41E-04	0.519
6.62E-04	0.830
1.10E-03	1.413
1.54E-03	1.979
2.21E-03	2.899



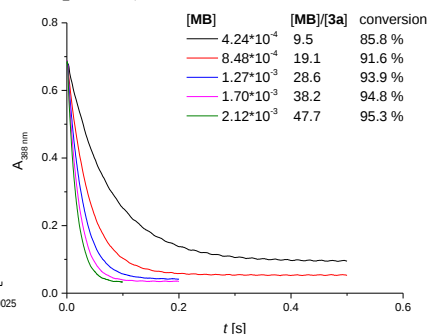
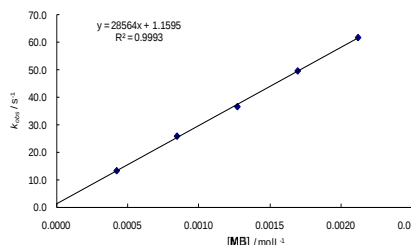
$$k_2 = 1340.2 \pm 11.28; C = -0.0684 \pm 0.015; \log k_2 = 3.13$$

reactions of **3a** show incomplete conversion (additionally given are the UV/vis spectra)

reactions of **3a** with **MB**

DMSO, 20 °C, stopped flow, 388 nm

[MB] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.24E-04	13.271
8.48E-04	25.902
1.27E-03	36.677
1.70E-03	49.737
2.12E-03	61.925



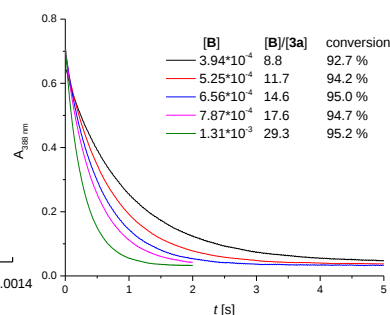
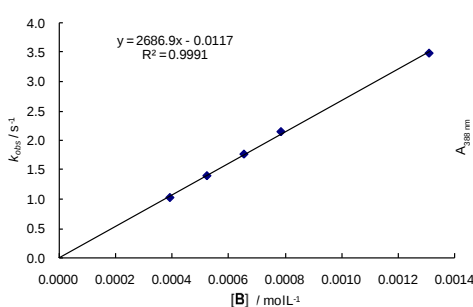
$$k_2 = 28564 \pm 429.95; C = 1.1595 \pm 0.6048; \log k_2 = 4.46$$

determined by incomplete conversions: $K = 12492 \text{ mol L}^{-1}$; $k_{-1} = 2.35 \text{ s}^{-1}$

reactions of **3a** with **B**

DMSO, 20 °C, stopped flow, 388 nm

[B] / M	$k_{\text{obs}} / \text{s}^{-1}$
3.94E-04	1.018
5.25E-04	1.392
6.56E-04	1.762
7.87E-04	2.147
1.31E-03	3.492



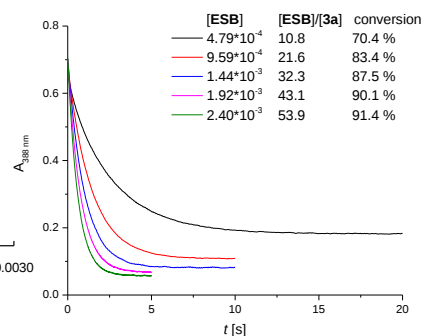
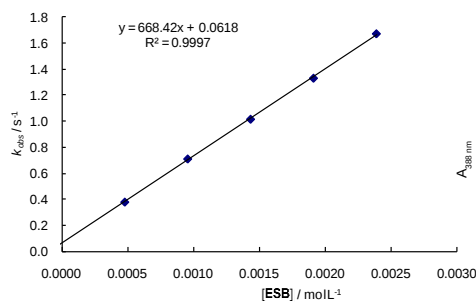
$$k_2 = 2686.9 \pm 46.80; C = -0.0117 \pm 0.0374; \log k_2 = 3.43$$

determined by incomplete conversions: $K = 28058 \text{ mol L}^{-1}$; $k_{-1} = 0.105 \text{ s}^{-1}$

reactions of **3a** with **ESB**

DMSO, 20 °C, stopped flow, 388 nm

[ESB] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.79E-04	0.381
9.59E-04	0.712
1.44E-03	1.017
1.92E-03	1.332
2.40E-03	1.673



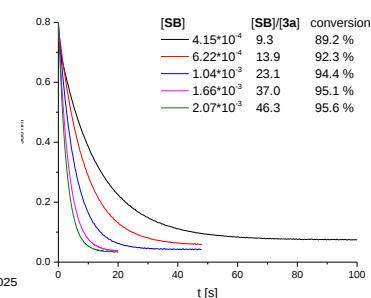
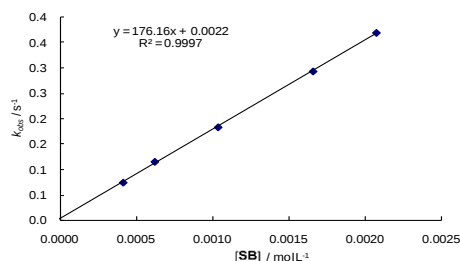
$$k_2 = 668.42 \pm 7.027; C = 0.0618 \pm 0.0112; \log k_2 = 2.83$$

determined by incomplete conversions: $K = 5021 \text{ molL}^{-1}$; $k_{-1} = 0.134 \text{ s}^{-1}$

reactions of **3a** with **SB**

DMSO, 20 °C, stopped flow, 388 nm

[SB] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.15E-04	0.074
6.22E-04	0.115
1.04E-03	0.183
1.66E-03	0.293
2.07E-03	0.369



$$k_2 = 176.16 \pm 1.834; C = 0.0022 \pm 0.0024; \log k_2 = 2.25$$

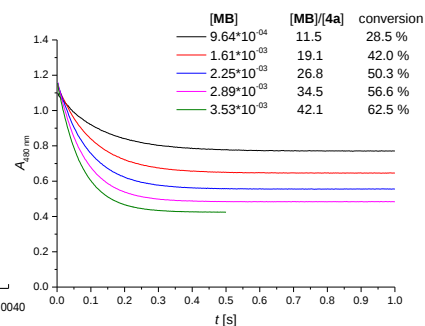
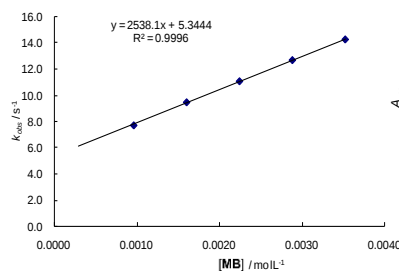
determined by incomplete conversions: $K = 16456 \text{ molL}^{-1}$; $k_{-1} = 0.0116 \text{ s}^{-1}$

reactions of **4a** show incomplete conversion (additionally given are the UV/vis spectra)

reactions of **4a** with **MB**

DMSO, 20 °C, stopped flow, 480 nm

[MB] / M	$k_{\text{obs}} / \text{s}^{-1}$
9.64E-04	7.726
1.61E-03	9.482
2.25E-03	11.084
2.89E-03	12.696
3.53E-03	14.273



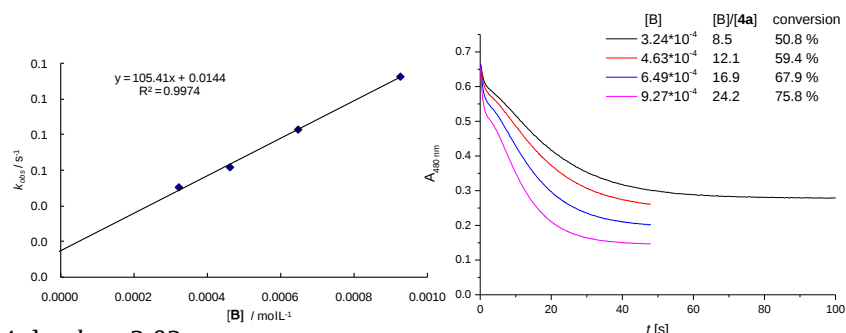
$$k_2 = 2538.1 \pm 29.379; C = 5.3444 \pm 0.071; \log k_2 = 3.40$$

determined by incomplete conversions: $K = 456 \text{ molL}^{-1}$; $k_{-1} = 5.58 \text{ s}^{-1}$

reactions of **4a** with **B**

DMSO, 20 °C, stopped flow, 480 nm

[B] / M	$k_{\text{obs}} / \text{s}^{-1}$
3.24E-04	0.050
4.63E-04	0.061
6.49E-04	0.083
9.27E-04	0.113



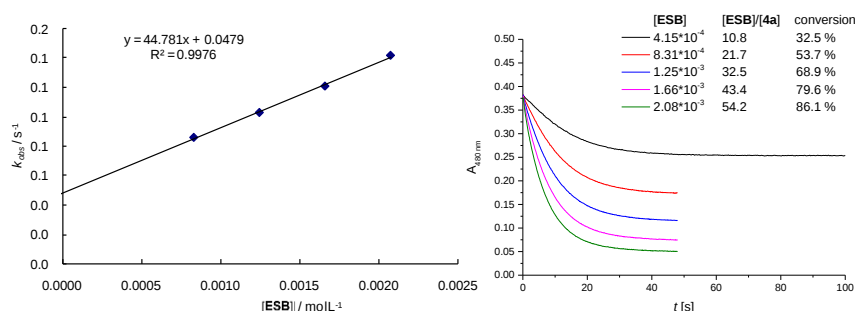
$$k_2 = 105.41 \pm 3.822; C = 0.0144 \pm 0.0024; \log k_2 = 2.02$$

determined by incomplete conversions: $K = 3399 \text{ molL}^{-1}$; $k_{-1} = 0.0309 \text{ s}^{-1}$

reactions of **4a** with **ESB**

DMSO, 20 °C, stopped flow, 480 nm

[ESB] / M	$k_{\text{obs}} / \text{s}^{-1}$
3.24E-04	0.050
4.63E-04	0.061
6.49E-04	0.083
9.27E-04	0.113



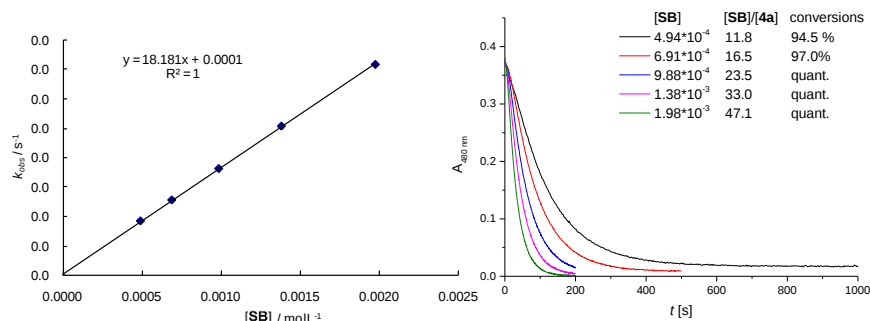
$$k_2 = 44.781 \pm 1.5603; C = 0.0479 \pm 0.0024; \log k_2 = 1.65$$

determined by incomplete conversions: $K = 2453 \text{ molL}^{-1}$; $k_{-1} = 0.0318 \text{ s}^{-1}$

reactions of **4a** with **SB**

DMSO, 20 °C, stopped flow, 480 nm

[SB] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.94E-04	0.009
4.246.91E-04	0.013
9.88E-04	0.018
1.38E-03	0.025
1.98E-03	0.036



$$k_2 = 18.181 \pm 0.0647; C = 0.0001 \pm 7.93 \cdot 10^{-5}; \log k_2 = 1.26$$

determined by incomplete conversions (2 lowest concentrations of SB):

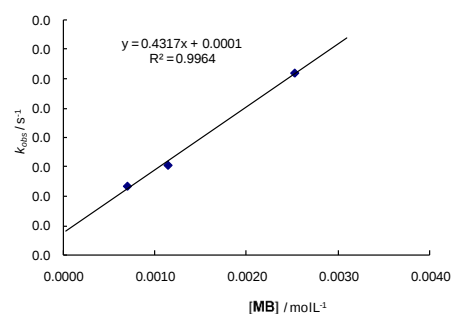
$$K = 43762 \text{ molL}^{-1}; k_{-1} = 0.000424 \text{ s}^{-1}$$

reactions of **5a**

reactions of **5a** with **MB**

DMSO, 20 °C, UV/vis cycle, 311 nm

[MB] / M	$k_{\text{obs}} / \text{s}^{-1}$
6.973E-04	0.0004684
1.140E-03	0.0006114
2.520E-03	0.00124098



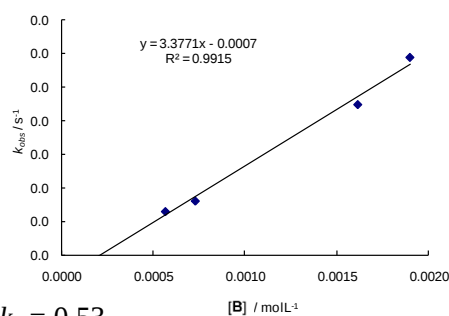
$$k_2 = 0.4317 \pm 0.0260; C = 0.0001 \pm 4.28 \cdot 10^{-5}; \log k_2 = -0.36$$

reactions of **5a** with **B**

DMSO, 20 °C, UV/vis cycle, 311 nm

[B] / M	$k_{\text{obs}} / \text{s}^{-1}$
5.620E-04	0.0013006
7.259E-04	0.0016130
1.615E-03	0.0044789
1.901E-03	0.0058811

$$k_2 = 3.3771 \pm 0.2211; C = -0.0007 \pm 2.94 \times 10^{-4}; \log k_2 = 0.53$$

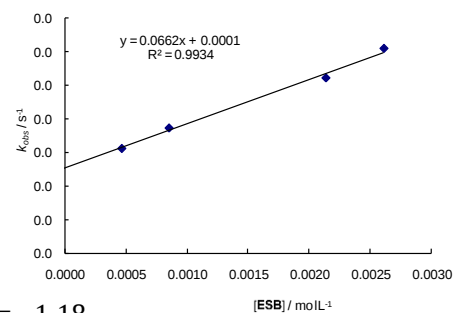


reactions of **5a** with **ESB**

DMSO, 20 °C, UV/vis cycle, 311 nm

[ESB] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.688E-04	0.0001566
8.548E-04	0.0001869
2.136E-03	0.0002611
2.610E-03	0.0003047

$$k_2 = 0.0662 \pm 0.0038; C = 0.0001 \pm 6.72 \times 10^{-6}; \log k_2 = -1.18$$

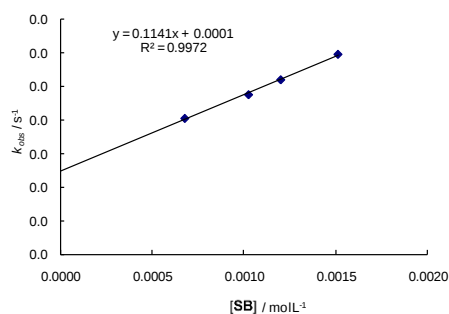


reactions of **5a** with **SB**

DMSO, 20 °C, UV/vis cycle, 311 nm

[SB] / M	$k_{\text{obs}} / \text{s}^{-1}$
6.755E-04	0.0002023
1.025E-03	0.0002376
1.201E-03	0.0002598
1.514E-03	0.0002978

$$k_2 = 0.1141 \pm 0.0043; C = 0.0001 \pm 4.89 \times 10^{-6}; \log k_2 = -0.94$$



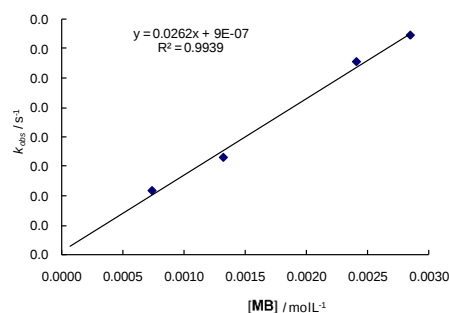
reactions of **5b**

reactions of **5b** with **MB**

DMSO, 20 °C, UV/vis cycle, 354 nm

[MB] / M	$k_{\text{obs}} / \text{s}^{-1}$
7.380E-04	0.000021642
1.321E-03	0.000032990
2.409E-03	0.000065710
2.849E-03	0.000074777

$$k_2 = 0.0262 \pm 0.0014; C = 8.88 \times 10^{-7} \pm 2.91 \times 10^{-6}; \log k_2 = -1.58$$

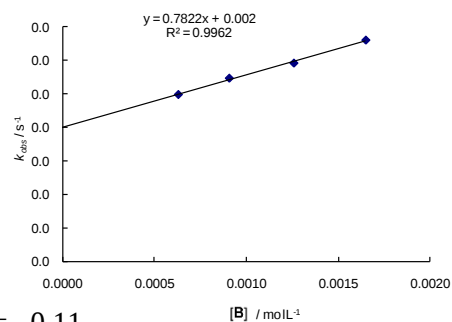


reactions of **5b** with **B**

DMSO, 20 °C, UV/vis cycle, 354 nm

[B] / M	$k_{\text{obs}} / \text{s}^{-1}$
6.278E-04	0.0024888
9.055E-04	0.0027336
1.257E-03	0.0029595
1.649E-03	0.0033041

$$k_2 = 0.7822 \pm 0.0343; C = 0.0020 \pm 4.02 \times 10^{-5}; \log k_2 = -0.11$$

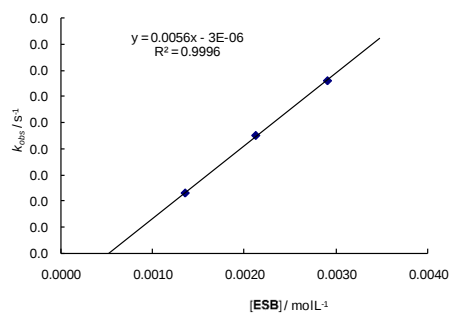


reactions of **5b** with **ESB**

DMSO, 20 °C, UV/vis cycle, 354 nm

[ESB] / M	$k_{\text{obs}} / \text{s}^{-1}$
1.350E-03	0.0000046
2.120E-03	0.0000090
2.903E-03	0.0000133

$$k_2 = 0.0056 \pm 1.08 \times 10^{-4}; C = -2.94 \times 10^{-6} \pm 2.39 \times 10^{-7}; \log k_2 = -2.25$$

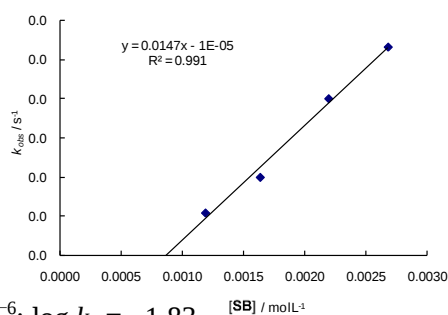


reactions of **5b** with **SB**

DMSO, 20 °C, UV/vis cycle, 354 nm

[SB] / M	$k_{\text{obs}} / \text{s}^{-1}$
1.188E-03	0.000005407
1.635E-03	0.000009957
2.194E-03	0.000020003
2.679E-03	0.000026599

$$k_2 = 0.0147 \pm 9.904 \times 10^{-4}; C = -1.28 \times 10^{-5} \pm 1.99 \times 10^{-6}; \log k_2 = -1.83$$



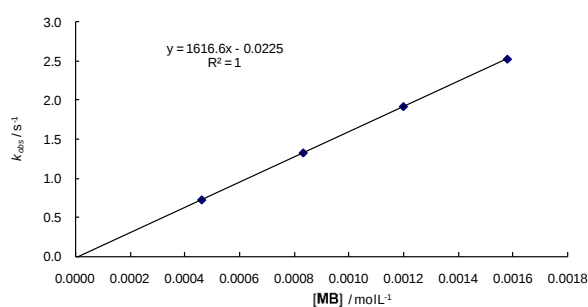
reactions of **6a**

reactions of **6a** with **MB**

DMSO, 20 °C, stopped flow, 422 nm

[MB] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.63E-04	0.724
8.34E-04	1.327
1.20E-03	1.921
1.58E-03	2.529

$$k_2 = 1616.6 \pm 4.878; C = -0.0225 \pm 0.0054; \log k_2 = 3.21$$

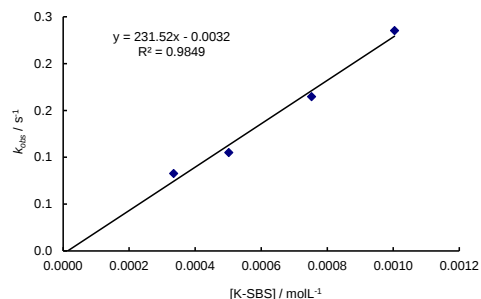


reactions of **6a** with **B**

DMSO, 20 °C, stopped flow, 422 nm

[B] / M	$k_{\text{obs}} / \text{s}^{-1}$
3.35E-04	0.083
5.02E-04	0.105
7.53E-04	0.165
1.00E-03	0.235

$$k_2 = 231.52 \pm 20.241; C = -0.0032 \pm 0.014; \log k_2 = 2.36$$

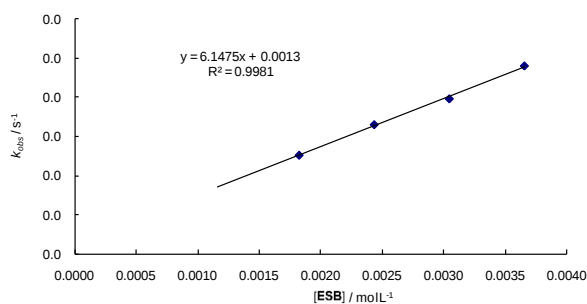


reactions of **6a** with **ESB**

DMSO, 20 °C, stopped flow, 422 nm

[ESB] / M	$k_{\text{obs}} / \text{s}^{-1}$
1.83E-03	0.0126
2.44E-03	0.0165
3.05E-03	0.0198
3.66E-03	0.0240

$$k_2 = 6.1475 \pm 0.1905; C = 0.0013 \pm 5.39 \times 10^{-4}; \log k_2 = 0.79$$

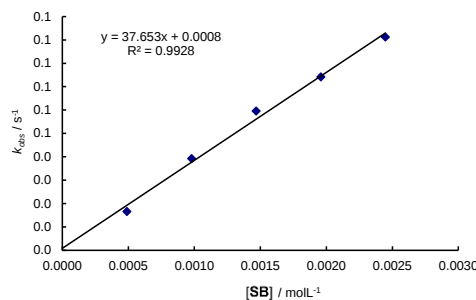


reactions of **6a** with **SB**

DMSO, 20 °C, stopped flow, 422 nm

[SB] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.89E-04	0.01311
9.79E-04	0.03272
1.47E-03	0.04904
1.96E-03	0.06848
2.45E-03	0.0863

$$k_2 = 37.653 \pm 1.853; C = 0.0008 \pm 0.003; \log k_2 = 1.58$$



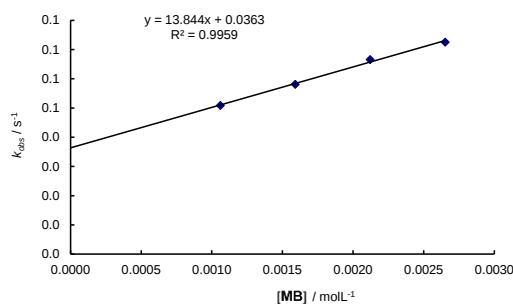
reactions of **6b**

reactions of **6b** with **MB**

DMSO, 20 °C, stopped flow, 533nm

[MB] / M	$k_{\text{obs}} / \text{s}^{-1}$
1.06E-03	0.0509
1.59E-03	0.0581
2.12E-03	0.0666
2.65E-03	0.0726

$$k_2 = 13.844 \pm 0.6278; C = 0.0363 \pm 0.0012; \log k_2 = 1.14$$

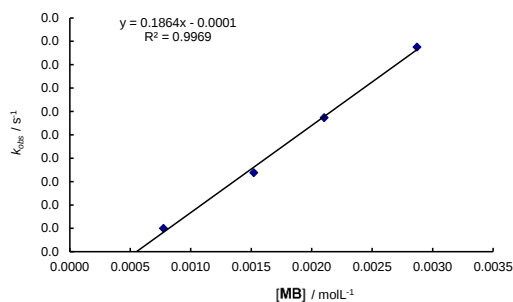


reactions of **6b** with **ESB**

DMSO, 20 °C, UV/vis cycle, 533nm

[ESB] / M	$k_{\text{obs}} / \text{s}^{-1}$
7.74E-04	0.0000501
1.52E-03	0.000169
2.10E-03	0.000287
2.87E-03	0.000438

$$k_2 = 0.1864 \pm 0.0072; C = -1.03 \times 10^{-4} \pm 1.41 \times 10^{-5}; \log k_2 = -0.73$$

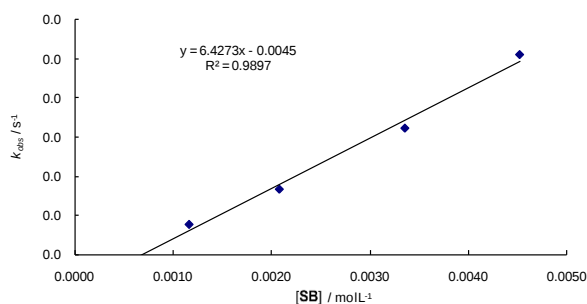


reactions of **6b** with **SB**

DMSO, 20 °C, UV/vis cycle, 533nm

[SB] / M	$k_{\text{obs}} / \text{s}^{-1}$
1.16E-03	0.0038
2.08E-03	0.0083
3.36E-03	0.0161
4.53E-03	0.0255

$$k_2 = 6.4273 \pm 0.4723; C = -0.0045 \pm 0.0014; \log k_2 = 0.81$$



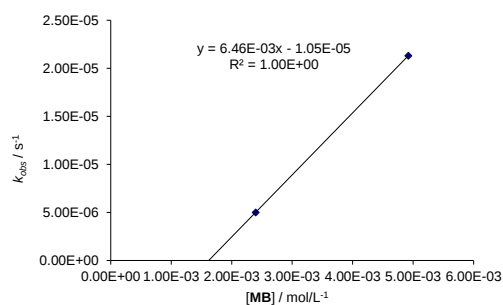
reactions of **6c**

reactions of **6c** with **MB**

DMSO, 20 °C, UV/vis cycle, 371nm

[MB] / M	$k_{\text{obs}} / \text{s}^{-1}$
2.397E-03	0.000005
4.921E-03	0.0000213

$$k_2 = 0.00646 \pm 0.0; C = 1.05 \times 10^{-5} \pm 0.0; \log k_2 = -2.19$$

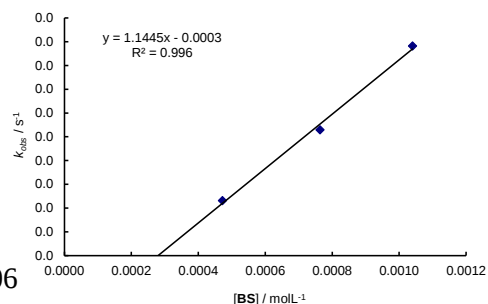


reactions of **6c** with **B**

DMSO, 20 °C, UV/vis cycle, 371nm

[B] / M	$k_{\text{obs}} / \text{s}^{-1}$
4.72E-04	2.31E-04
7.63E-04	5.29E-04
1.04E-03	0.00088195

$$k_2 = 1.1445 \pm 0.072; C = -0.0003 \pm 5.72 \times 10^{-5}; \log k_2 = 0.06$$



Kinetics of a Nucleophile electrophil reaction with a subsequent proton transfer:

Independently of the real mechanism of the PT-reaction, this process is considered as first-order-reaction with respect to its stoichiometry. The suggested scenario, which includes the equilibrium of the C–C-bond formation and the subsequent PT-reaction, is shown in eq. S1



The rate law for the Bodenstein approximation (steady state of the initially formed adduct: $\text{N-E}^{\ominus}$) is given in eq. S2.

$$d[\text{N-E}^{\ominus}]/dt = k_2[\text{E}][\text{N}^{\ominus}] - k_{-1}[\text{N-E}^{\ominus}] - k_{PT}[\text{N-E}^{\ominus}] + k_{-PT}[{}^{\ominus}\text{N-E}] = 0 \quad (\text{S2})$$

If the equilibrium between $\text{N-E}^{\ominus}$ and ${}^{\ominus}\text{N-E}$ lies on the side of ${}^{\ominus}\text{N-E}$, than it could be stated that $k_{PT}[\text{N-E}^{\ominus}] \gg k_{-PT}[{}^{\ominus}\text{N-E}]$. From this assumption eq. S3 could be formulated.

$$d[\text{N-E}^{\ominus}]/dt = k_2[\text{E}][\text{N}^{\ominus}] - k_{-1}[\text{N-E}^{\ominus}] - k_{PT}[\text{N-E}^{\ominus}] = 0 \quad (\text{S3})$$

$$\text{This means } [\text{N-E}^{\ominus}] = k_2[\text{E}][\text{N}^{\ominus}]/(k_{-1} + k_{PT}) \quad (\text{S4})$$

For negligible concentrations of the intermediate $[\text{N-E}^{\ominus}]$, the rate of formation of the final product $[{}^{\ominus}\text{N-E}]$ equals the rate of consumption of the electrophile, as shown in eq. S5, where k_{-PT} is neglected because the conversion of $\text{N-E}^{\ominus}$ into ${}^{\ominus}\text{N-E}$ is quantitative.

$$-d[\text{E}]/dt = d[{}^{\ominus}\text{N-E}]/dt = k_{PT}[\text{N-E}^{\ominus}] \quad (\text{S5})$$

Substitution of eq. S4 into eq. S5 yields eq. S6

$$d[\text{E}]/dt = -k_2[\text{E}][\text{N}^{\ominus}] (k_{PT}/(k_{PT} + k_{-1})) \quad (\text{S6})$$

For $k_{PT} \gg k_{-1}$, eq. S6 simplifies to eq. S7

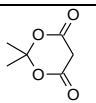
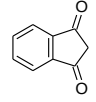
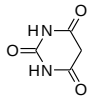
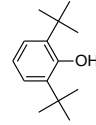
$$d[\text{E}]/dt = -k_2[\text{E}][\text{N}^{\ominus}] \quad (\text{S7})$$

and for $k_{PT} \ll k_{-1}$, eq. S6 transforms to eq. S8

$$d[\text{E}]/dt = -k_2[\text{E}][\text{N}^{\ominus}] (k_{PT}/k_{-1}) = -k_{PT}K [\text{E}][\text{N}^{\ominus}] = k_{app} [\text{E}][\text{N}^{\ominus}] \quad (\text{S8})$$

with $K = k_2/k_{-1}$

Table S2. Corresponding acids of the investigated *Michael*-acceptor electrophiles and their pK_a -values in DMSO.

corresponding Acid	pK_a (DMSO)
	Meldrum's Acid
	Indandione
	Barbituric Acid
	Malononitrile
	2,6-Di- <i>tert</i> -butylphenol

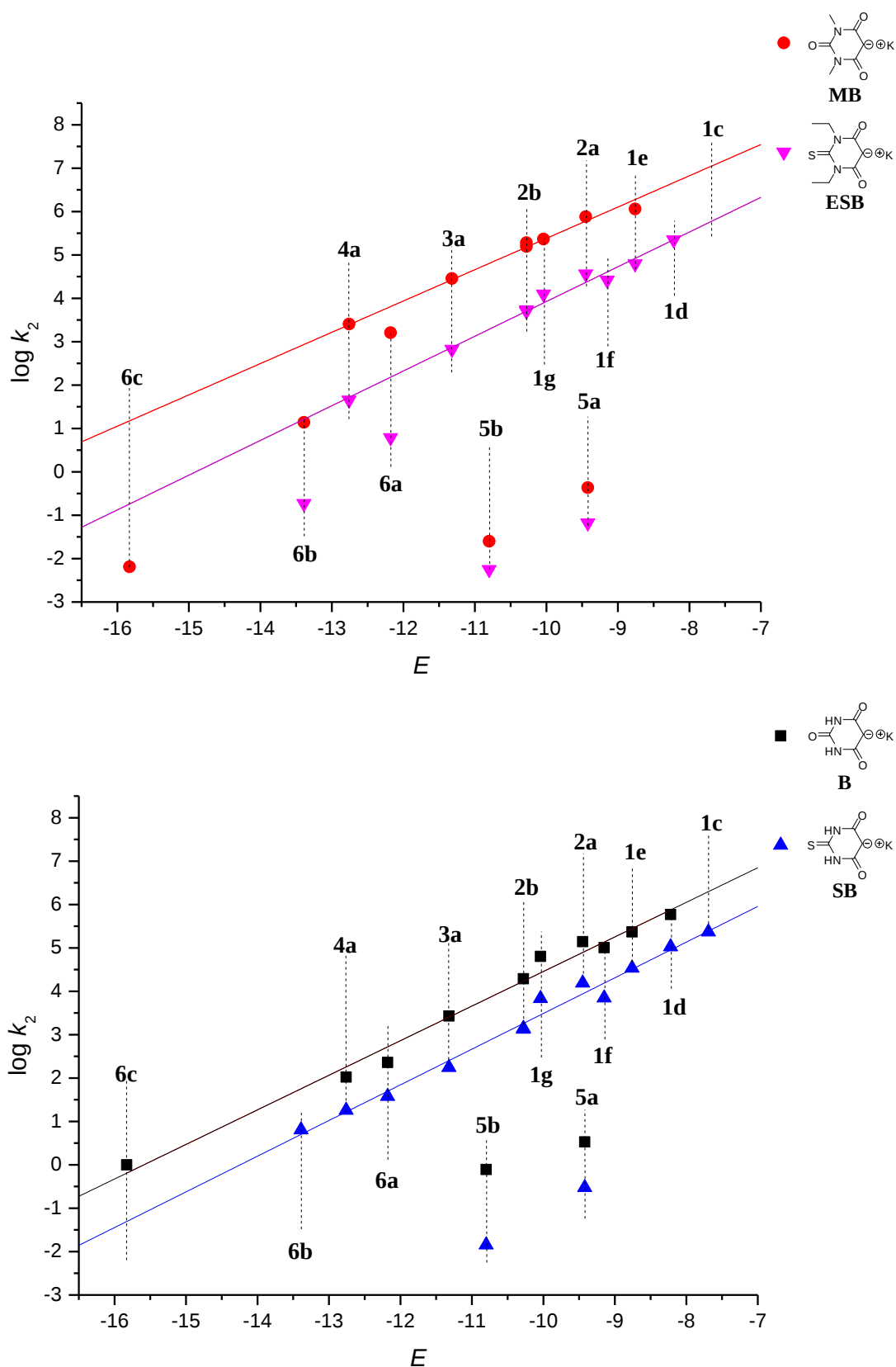


Figure S1. Comparison of alkylated oxo- and thiobarbituric anions (**MB**, **ESB**) at the top and unalkylated oxo- and thiobarbituric anions (**B**, **SB**) at the bottom, for better visualization of the slower rate constants (k_2) of thiobarbiturate anions.

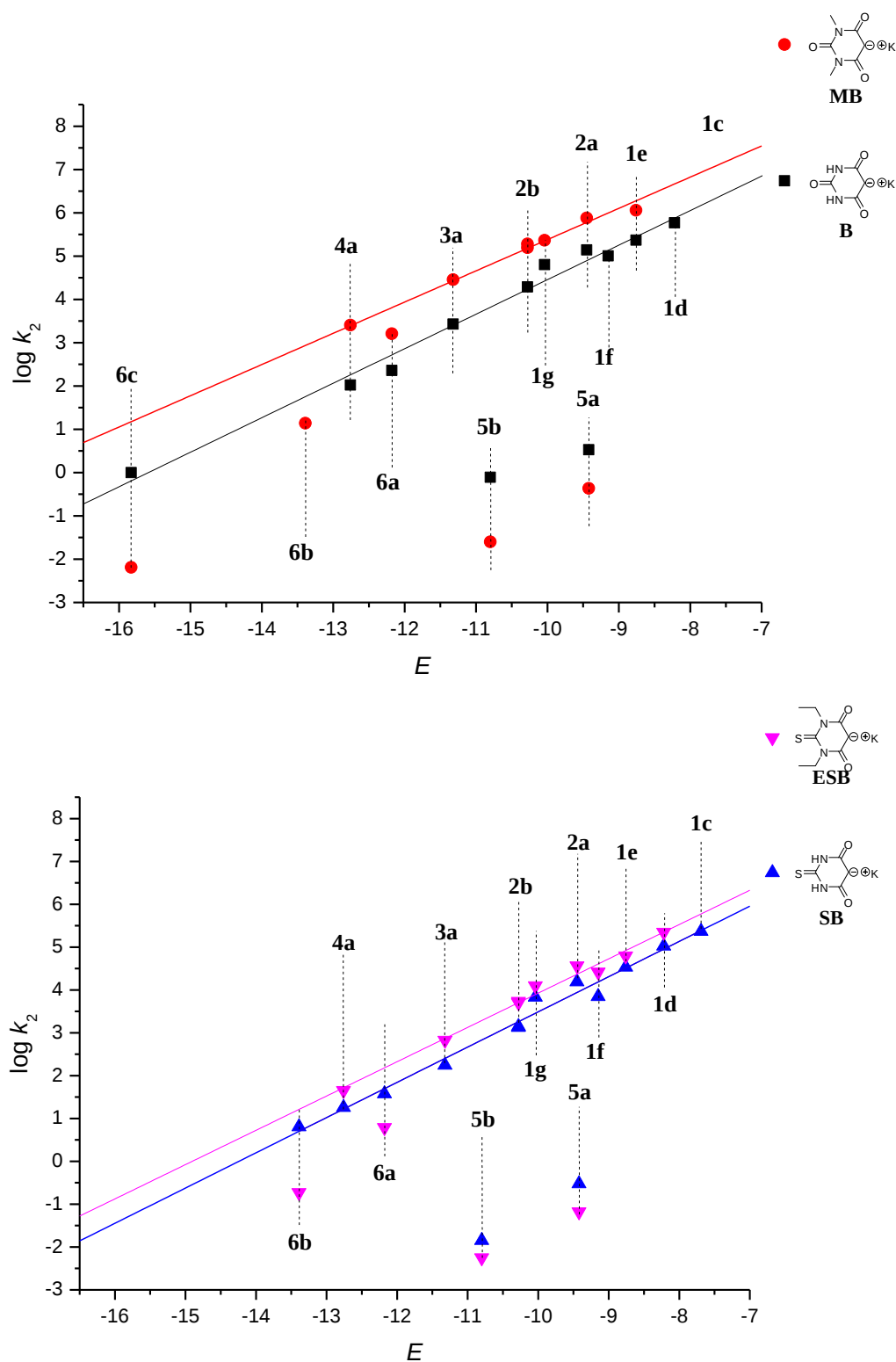
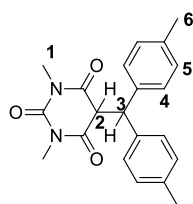


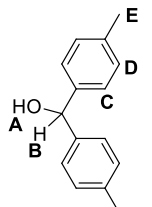
Figure S2. Comparison of alkylated and unalkylated oxobarbituric anions (**B**, **MB**) at the top and alkylated and unalkylated thiobarbituric anions (**SB**, **ESB**) at the bottom, for better visualization of the faster rate constants (k_2) through alkylation of barbiturate anions. Notable is the inverse substituent effect for the kinetics of electrophiles 5a and 5b, caused by the invers substituent effects on the proton transfer reaction.

NMR-Spectra – Product studies

MB1a:

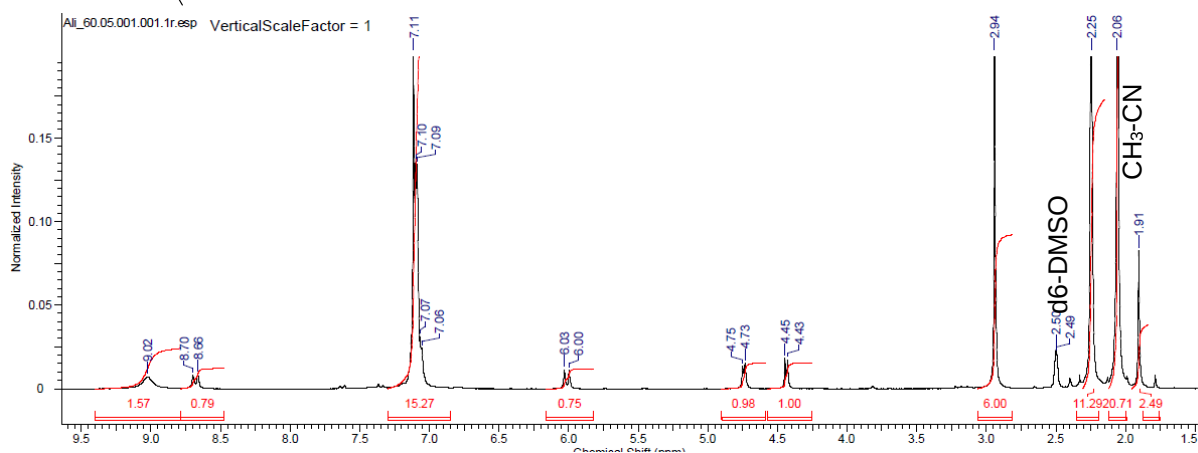


¹H NMR (d₆-DMSO): δ = 2.24 (s, 6H, ⁶CH₃), 2.94 (s, 6H, ¹CH₃), 4.44 (d, ³J_{HH} = 4.5 Hz, 1H, ³CH), 4.74 (d, ³J_{HH} = 4.5 Hz, 1H, ²CH), 7.06-7.13 (m, 8H, ⁴CH, ⁵CH)

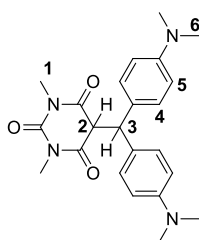


Side product (hydrolysis): Di-*p*-tolylmethanone

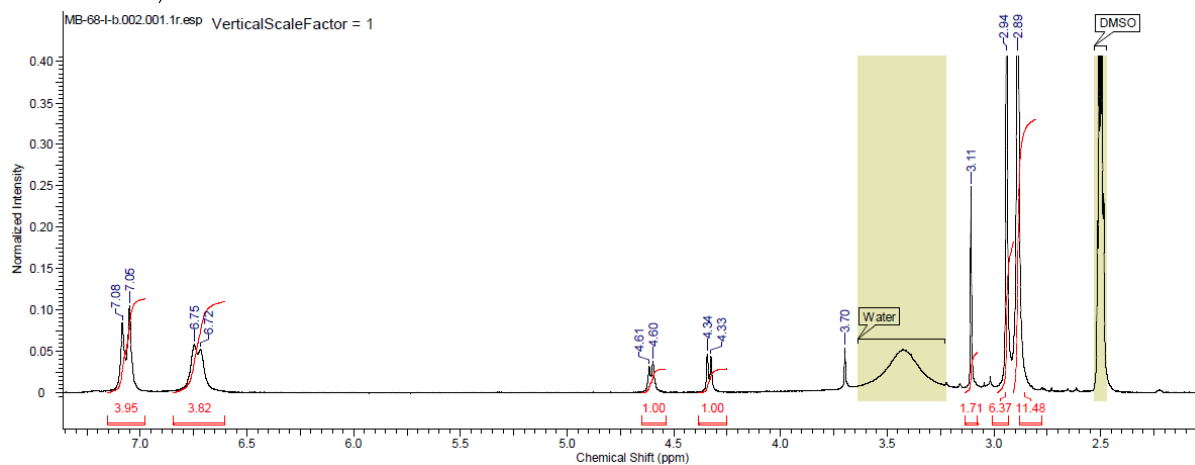
¹H NMR (d₆-DMSO): δ = 2.25 (s, 6H, ^ECH₃), 6.02 (d, ³J_{HH} = 8.5 Hz, 1H, ^AOH), 7.06-7.13 (m, 8H, ^CCH, ^DCH), 8.68 (d, ³J_{HH} = 8.8 Hz, 1H, ^BCH),



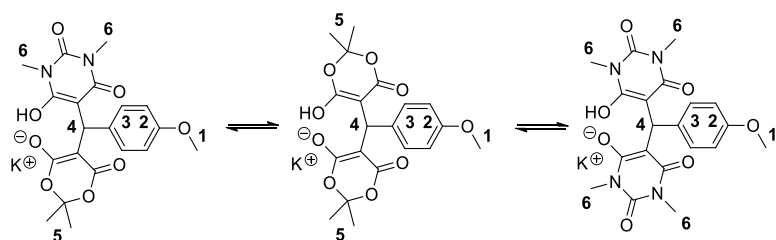
MB1b:



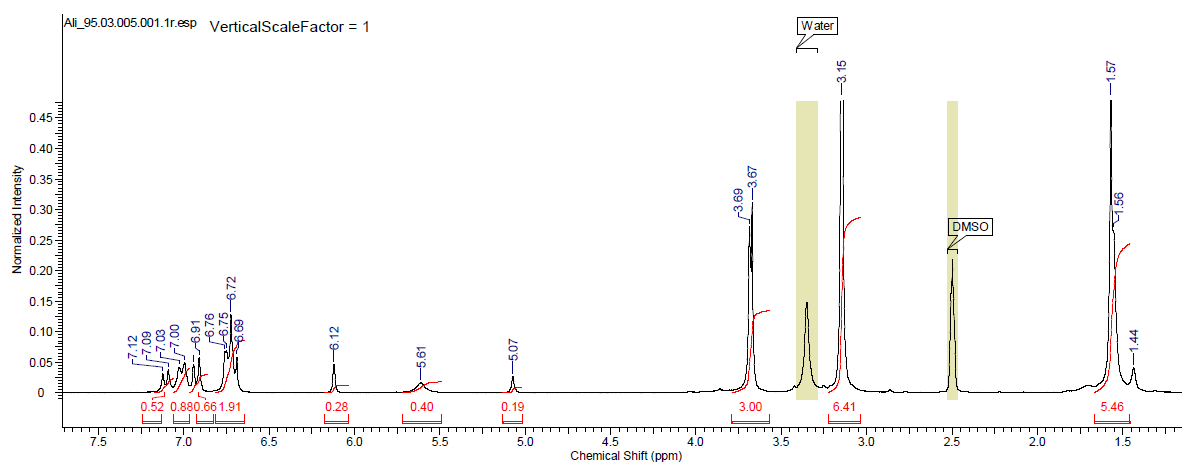
¹H NMR (d₆-DMSO): δ = 2.89 (s, 12H, ⁶CH₃), 2.94 (s, 6H, ¹CH₃), 4.33 (d, ³J_{HH} = 4.5 Hz, 1H, ³CH), 4.60 (d, ³J_{HH} = 4.5 Hz, 1H, ²CH), 6.74 (d, ³J_{HH} = 7.9 Hz, 4H, ⁵CH), 7.07 (d, ³J_{HH} = 7.9 Hz, 4H, ⁴CH)



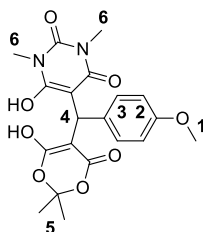
MB2b:



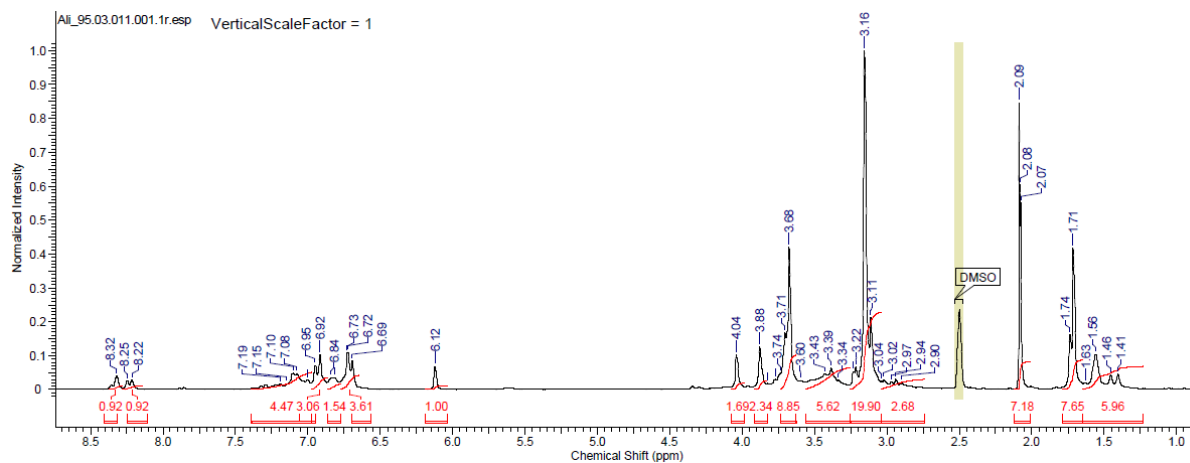
^1H NMR (d_6 -DMSO – Enol): δ 1.57 (s, 6H, $^5\text{CH}_3$), 3.15 (s, 6H, $^6\text{CH}_3$), 3.67, 3.69 (s, 3H, $^1\text{CH}_3$), [5.07 (s, 0.19H), 5.61 (s, 0.39H), 6.12 (s, 0.29H), $\Sigma = 1\text{H}$, ^4CH], [6.72 (m, 2H, ^2CH), 6.92 (d, $^3J_{\text{HH}} = 8.50$ Hz, 0.69H), 7.01 (d, $^3J_{\text{HH}} = 8.00$ Hz, 0.91H), 7.11 (d, $^3J_{\text{HH}} = 8.50$ Hz, 0.51H) $\Sigma = 2\text{H}$, ^3CH]

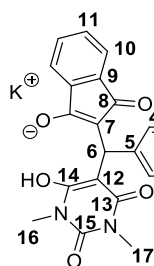


MB2b-H:



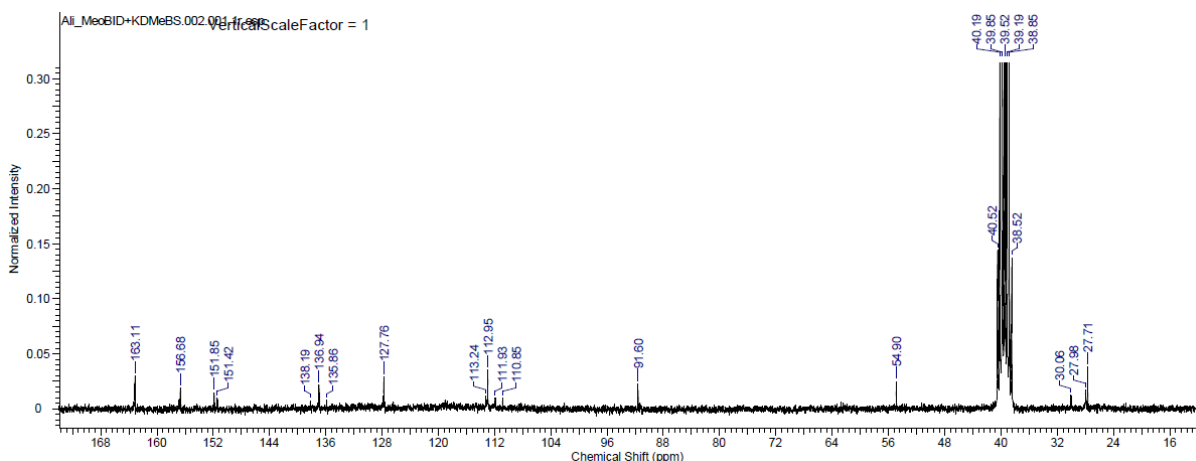
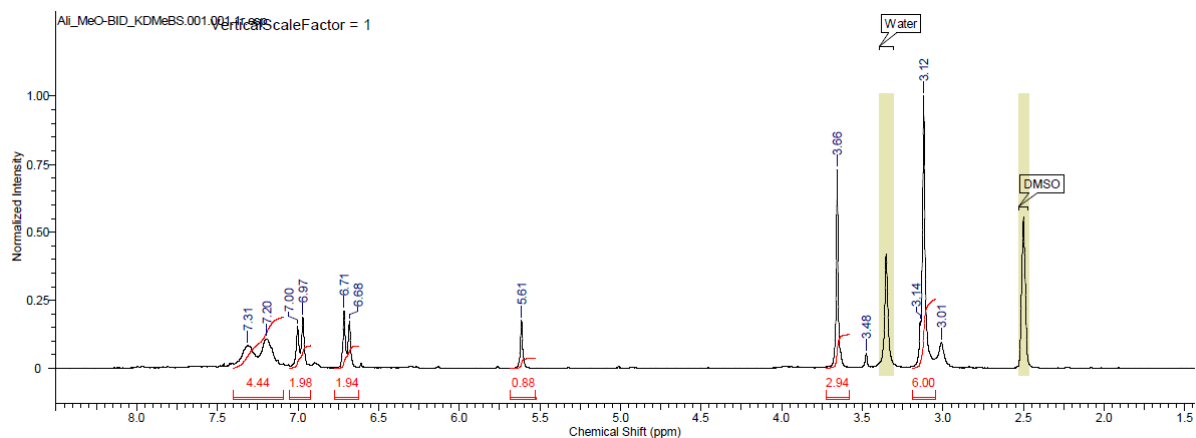
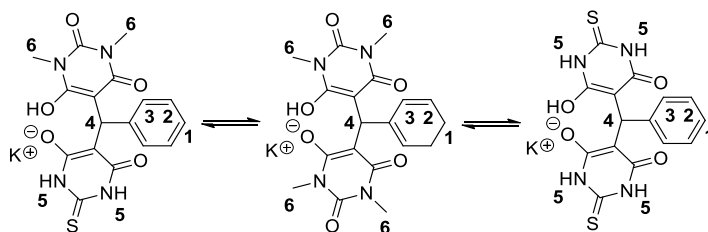
^1H NMR (d_6 -DMSO – Enol): δ 1.56 (s, 6H, $^5\text{CH}_3$), 3.16 (s, 6H, $^6\text{CH}_3$), 3.68 (s, 3H, $^1\text{CH}_3$), 6.12 (s, 1H, ^4CH), 6.71 (d, $^3J_{\text{HH}} = 7.25$ Hz, 2H, ^2CH), 6.93 (d, $^3J_{\text{HH}} = 8.25$ Hz, 2H, ^3CH)



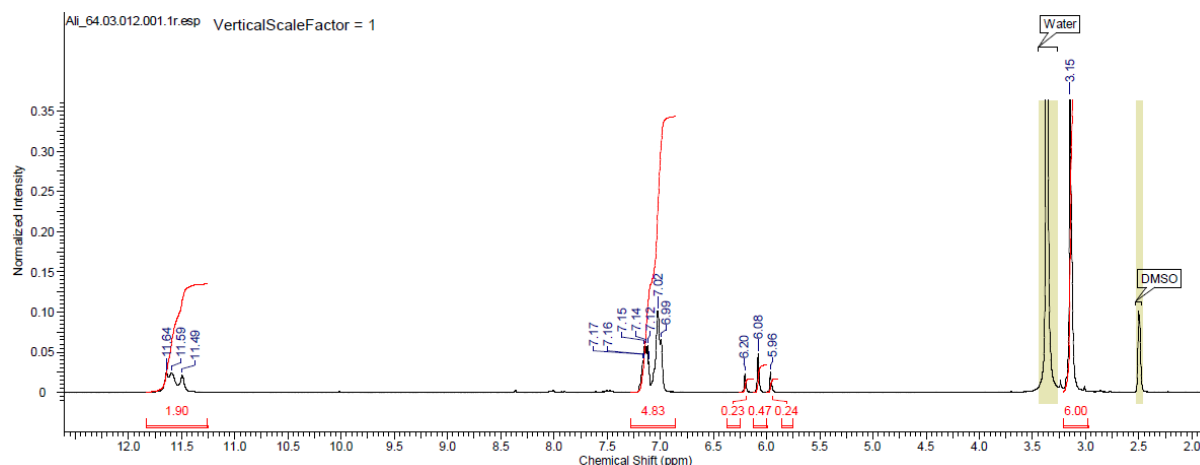
MB3a:

^1H NMR (d_6 -DMSO – Enol): δ 3.12 (s, 6H, $^{16,17}\text{CH}_3$), 3.66 (s, 3H, $^1\text{CH}_3$), 5.61 (s, 1H, ^6CH), 6.69 (d, $^3J_{\text{HH}} = 8.50$ Hz, 2H, ^3CH), 6.98 (d, $^3J_{\text{HH}} = 8.25$ Hz, 2H, ^4CH), 7.20–7.31 (m, 4H, $^{10,11}\text{CH}$)

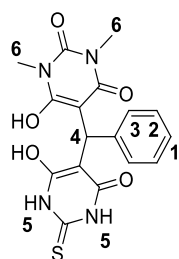
^{13}C NMR (d_6 -DMSO – Enol): δ 27.7, 28.0, 30.1 (^6CH , $^{16,17}\text{CH}_3$), 54.9 ($^1\text{CH}_3$), 91.6 (^7C), 110.9, 111.9, 113.0, 113.2, 127.8, 135.9, 136.9, 138.2 ($^{2,3,4,5,9,10,11,12}\text{C}$), 151.4, 151.9, 156.7, 163.1 ($^{8,13,14,15}\text{CO}$)

**SB4a:**

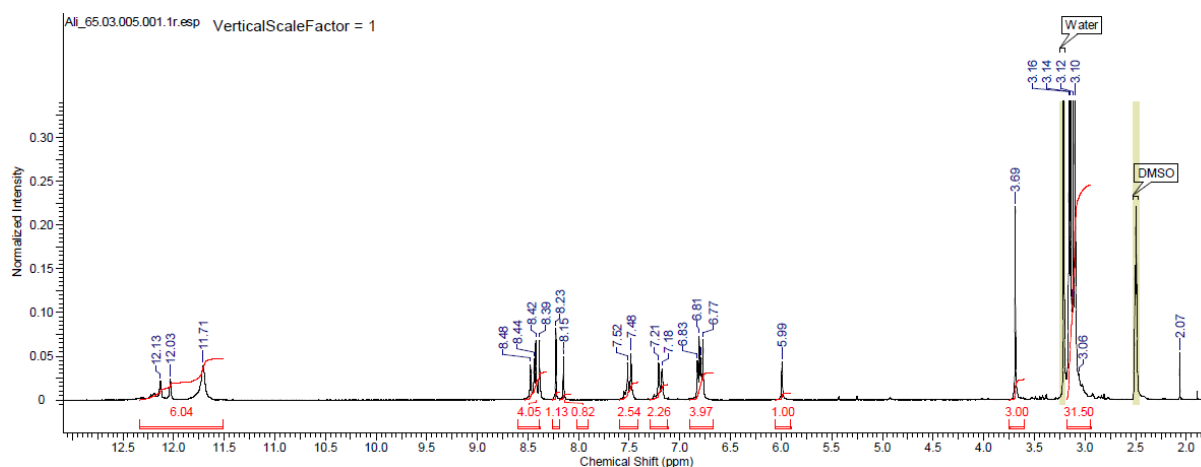
^1H NMR (d_6 -DMSO – Enol): δ 3.15 (s, 6H, $^6\text{CH}_3$), [5.97 (s, 0.24H), 6.08 (s, 0.49H), 6.21 (s, 0.25H) Σ 1H, ^4CH], 6.99–7.17 (m, 5H, $^{1,2,3}\text{CH}$), 11.59 (m, 2H, ^5NH)



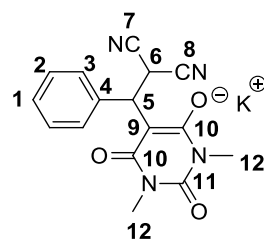
SB4a-H



^1H NMR (d_6 -DMSO – Enol): δ 3.10 (s, 6H, $^6\text{CH}_3$), 5.94 (s, 1H, ^4CH), 7.01–7.20 (m, 5H, $^{1,2,3}\text{CH}$), 11.74 (m, 2H, ^5NH)

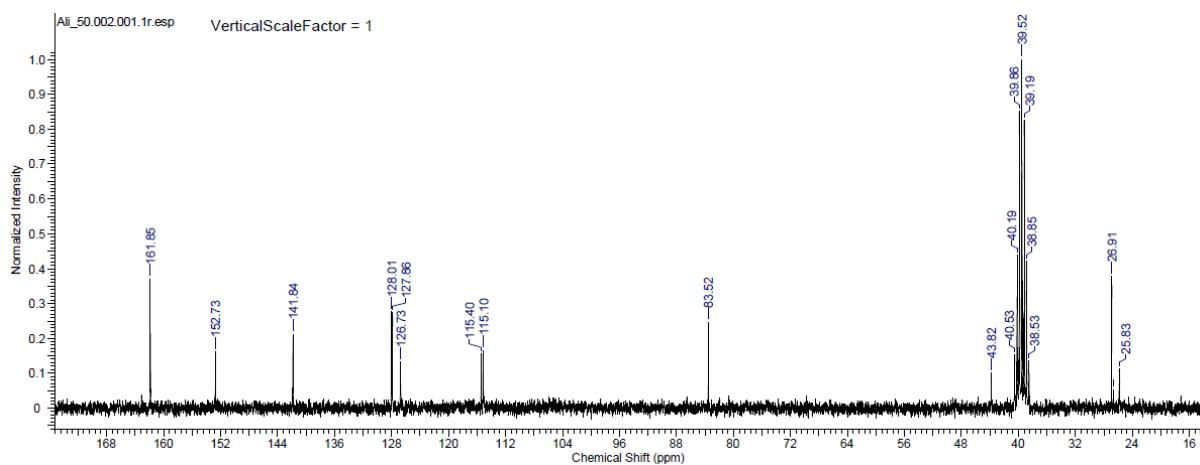
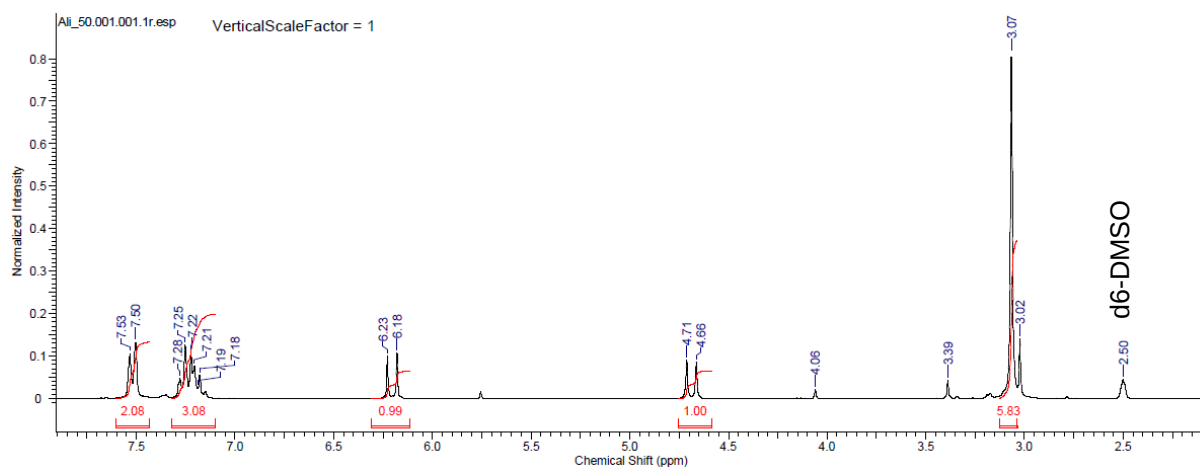


MB5a:

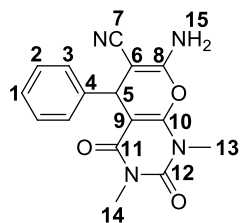


^1H NMR (d_6 -DMSO): δ 3.07 (s, 6H, $^{12}\text{CH}_3$), 4.69 (d, $^3J_{\text{HH}} = 12.25$ Hz, 1H, ^5CH), 6.20 (d, $^3J_{\text{HH}} = 12.25$ Hz, 1H, ^6CH), 7.18–7.28 (m, 3H, $^{1,2}\text{CH}$), 7.52 (d, $^3J_{\text{HH}} = 7.00$ Hz, 2H, ^3CH)

^{13}C NMR (d_6 -DMSO): δ 25.8 (^6CH), 26.9 ($^{12}\text{CH}_3$), 43.8 (^5CH), 83.5 (^9C), 115.1, 115.4 ($^{7,8}\text{CN}$), 126.7, 127.9, 128.0 ($^{1,2,3}\text{CH}$), 141.8 (^4C), 152.7 (^{11}CO), 161.9 (^{10}CO)

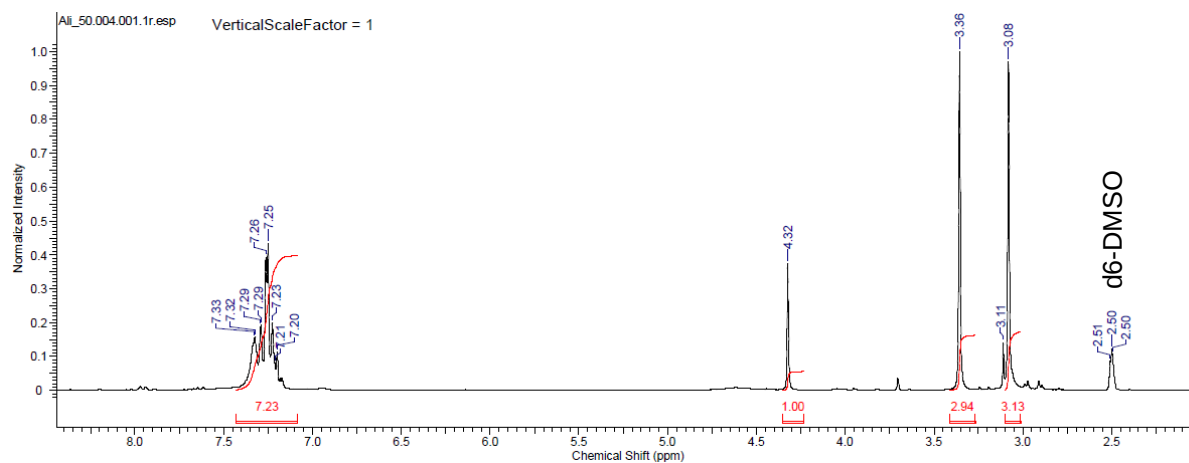


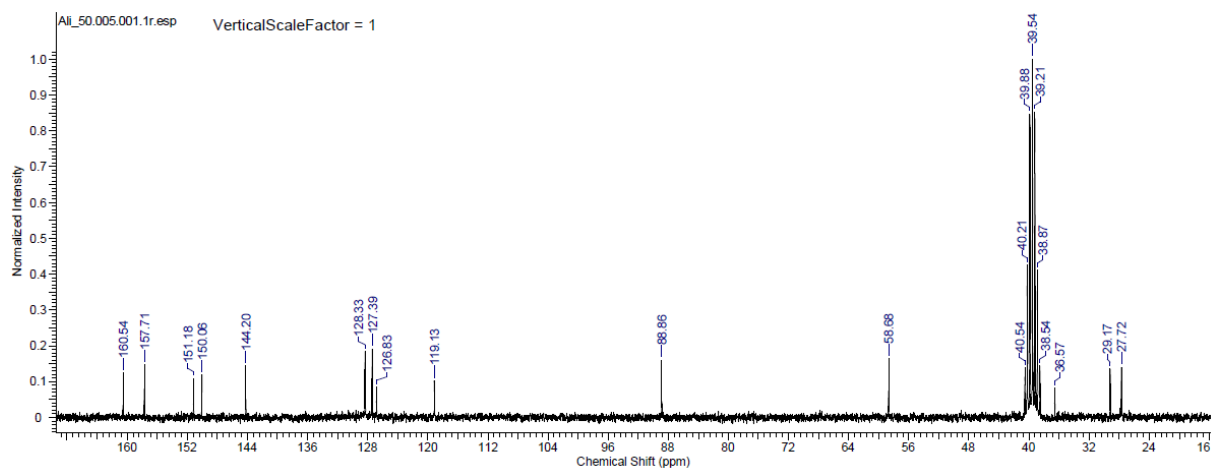
MB5a-H:



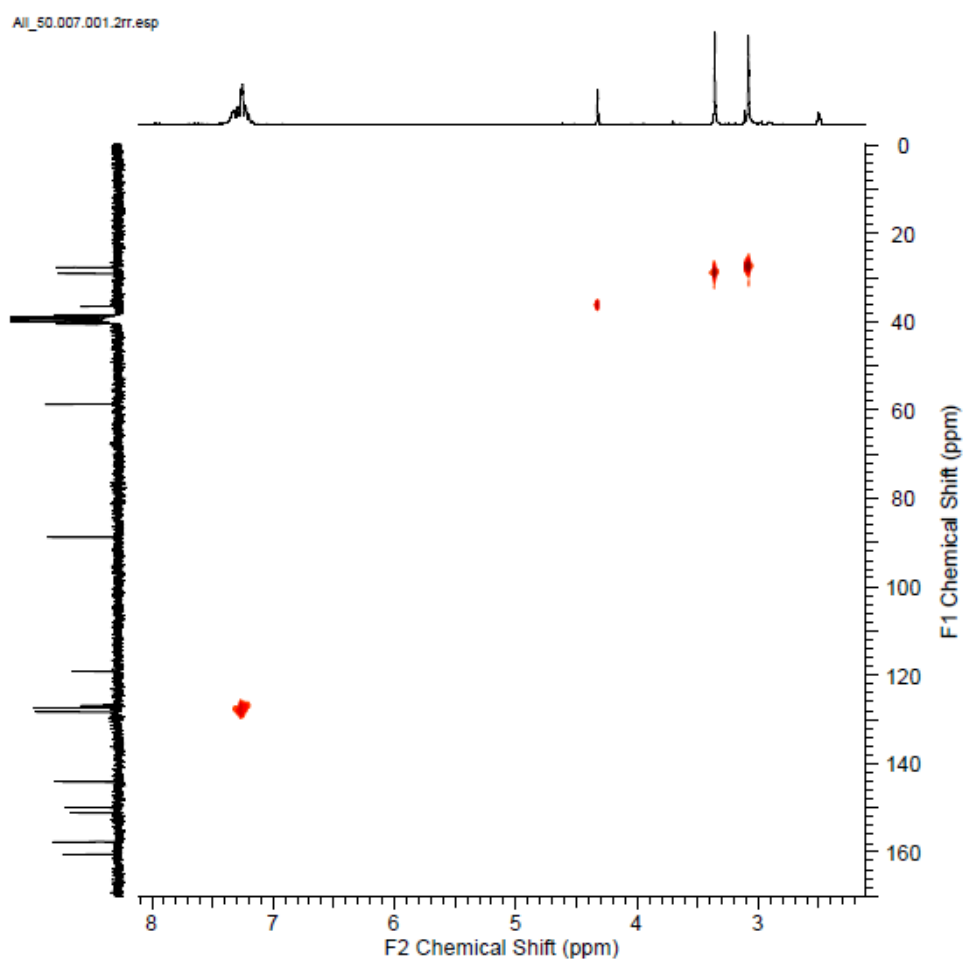
^1H NMR (d₆-DMSO): δ 3.08 (s, 3H, $^{14}\text{CH}_3$), 3.36 (s, 3H, $^{13}\text{CH}_3$), 4.32 (s, 1H, ^5CH), 7.20–7.33 (m, 7H, $^{1,2,3}\text{CH}$, $^{15}\text{NH}_2$)

^{13}C NMR (d₆-DMSO): δ 27.7 ($^{14}\text{CH}_3$), 29.2 ($^{13}\text{CH}_3$), 36.6 (^5CH), 58.7 (^6C), 88.9 (^9C), 119.1 (^7CN), 126.8, 127.4, 128.3 ($^{1,2,3}\text{CH}$), 144.2 (^4C), 150.1 (^{12}CO), 151.2 (^{10}C), 157.7 (^8C), 160.5 (^{11}CO)

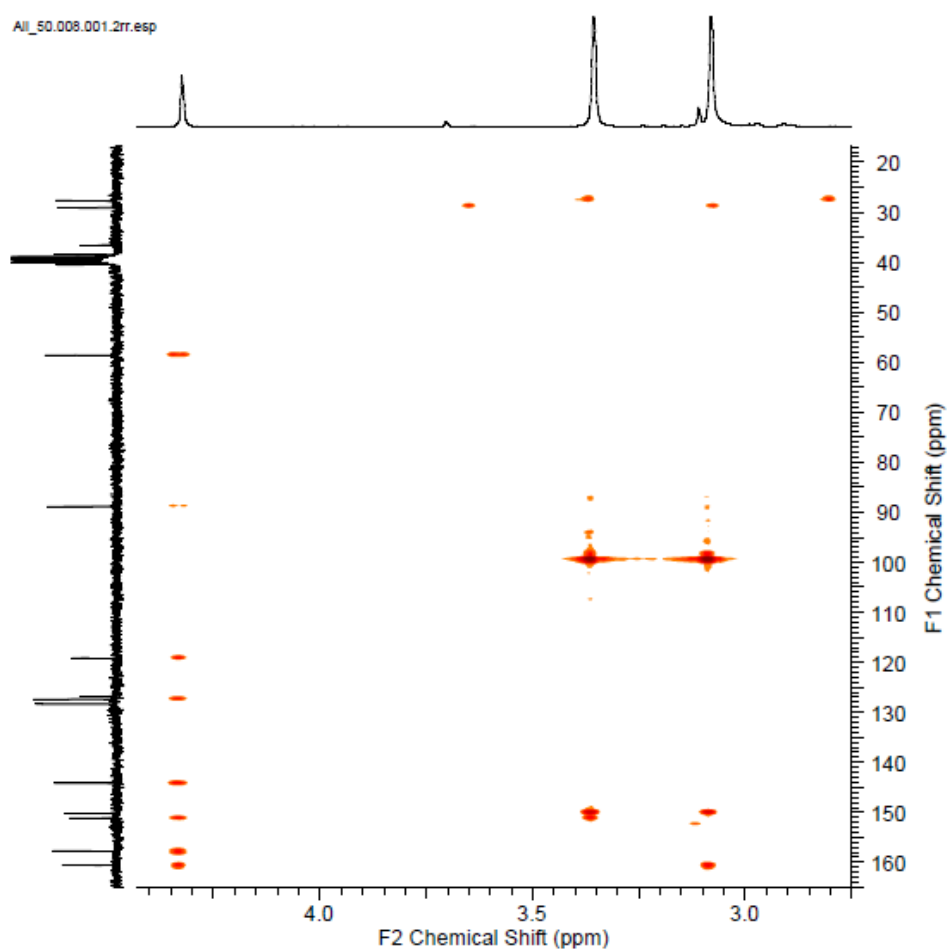




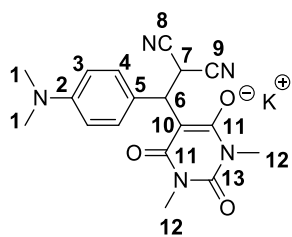
^1H - ^{13}C gs-HSQC:



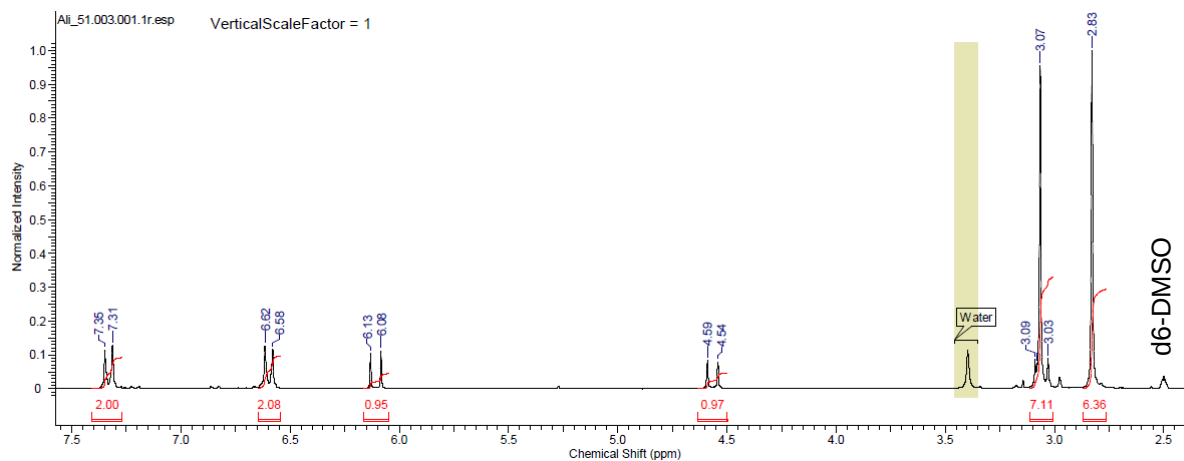
^1H - ^{13}C gs-HMBC:

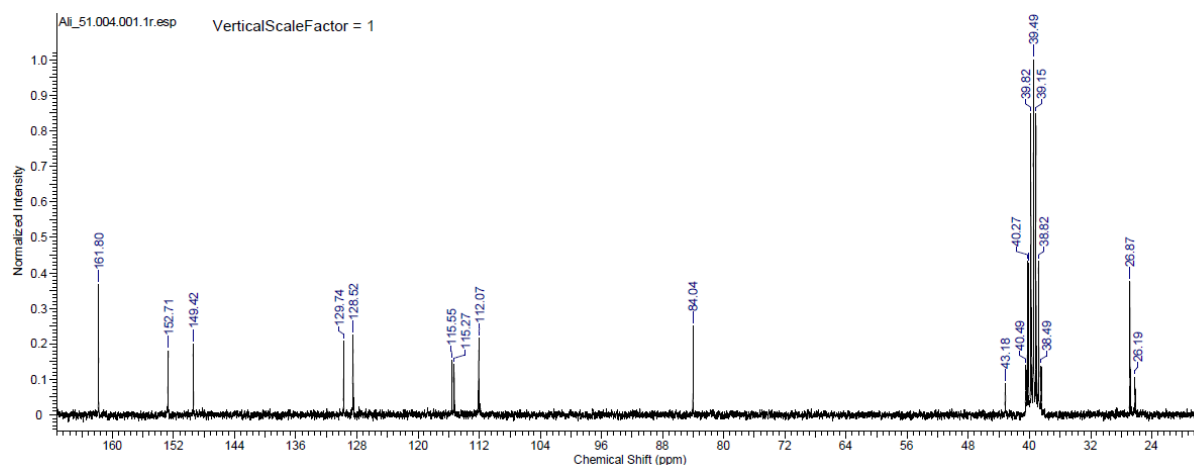


MB5c:

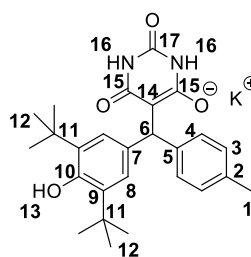


^1H NMR (d_6 -DMSO): δ 2.83 (s, 6H, $^1\text{CH}_3$), 3.07 (s, 6H, $^{12}\text{CH}_3$), 4.57 (d, $^3J_{\text{HH}} = 12.25$ Hz, 1H, ^6CH), 6.11 (d, $^3J_{\text{HH}} = 12.00$ Hz, 1H, ^7CH), 6.60 (d, $^3J_{\text{HH}} = 8.75$ Hz, 2H, ^3CH), 7.33 (d, $^3J_{\text{HH}} = 8.75$ Hz, 2H, ^4CH)
 ^{13}C NMR (d_6 -DMSO): δ 26.2 (^7CH), 26.9 ($^{12}\text{CH}_3$), 40.3 ($^1\text{CH}_3$), 43.2 (^6CH), 84.0 (^{10}C), 112.1 (^3CH), 115.3, 115.6 ($^{8,9}\text{CN}$), 128.5 (^4CH), 129.7 (^5C), 149.4 (^2C), 152.7 (^{13}CO), 161.8 (^{11}CO)

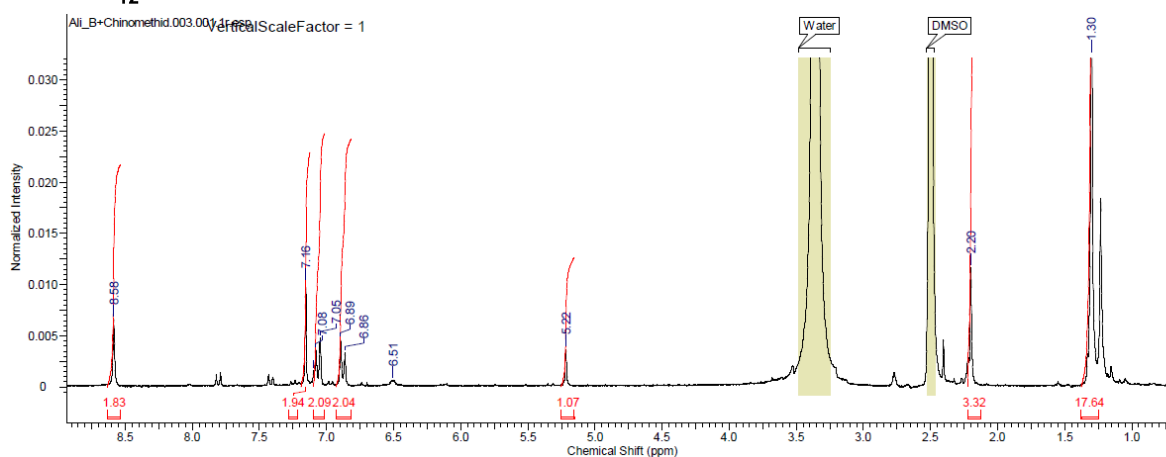




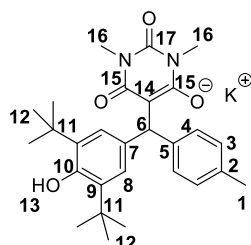
B6c:



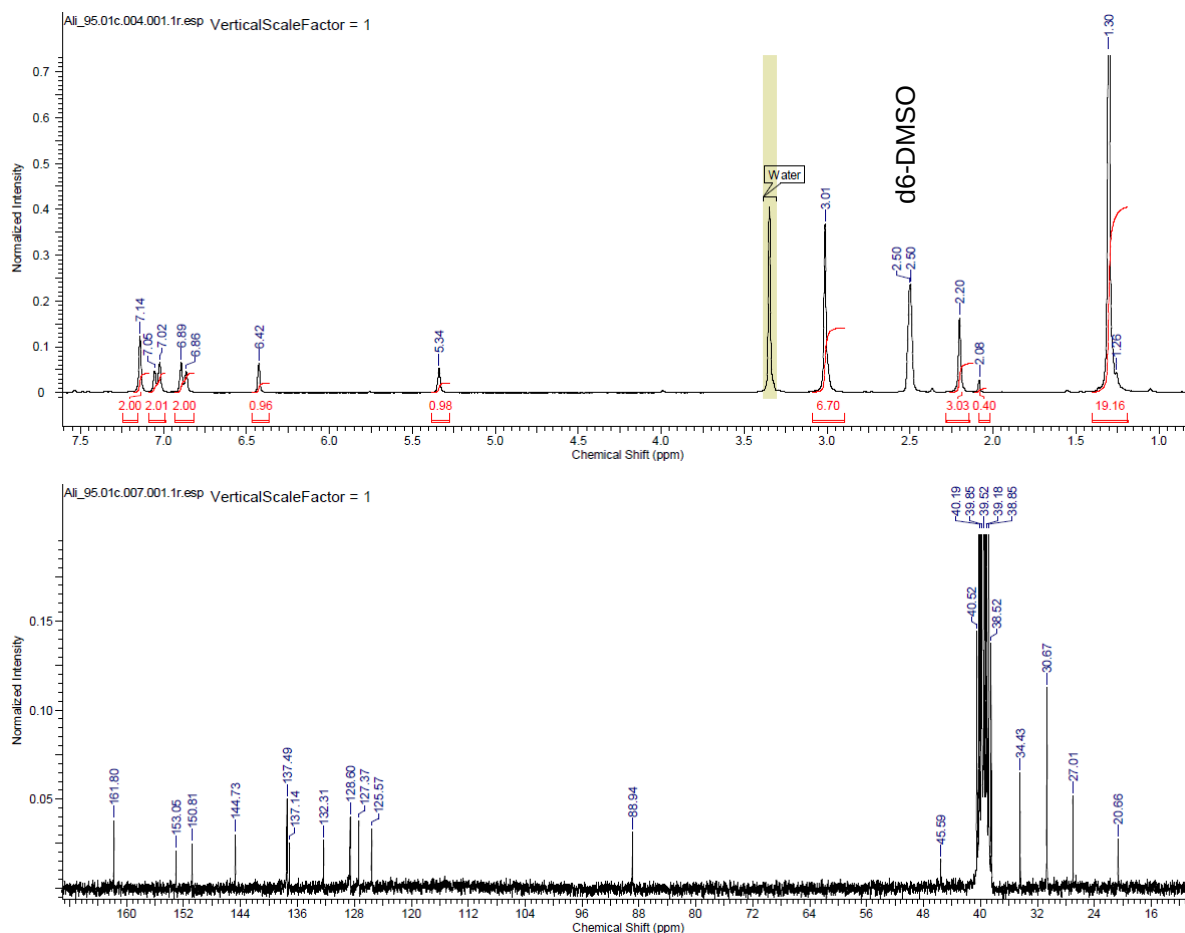
^1H NMR (d_6 -DMSO): δ 1.30 (s, 18H, $^{12}\text{CH}_3$), 2.20 (s, 3H, $^1\text{CH}_3$), 5.22 (s, 1H, ^6CH), 6.51 (s, 1H, ^{13}OH), 6.88 (d, $^3J_{\text{HH}} = 8.0$ Hz, 2H, $^{3/4}\text{CH}$), 7.07 (d, $^3J_{\text{HH}} = 8.0$ Hz, 2H, $^{3/4}\text{CH}$), 7.16 (s, 2H, ^8CH), 8.58 (s, 2H, ^{16}NH)



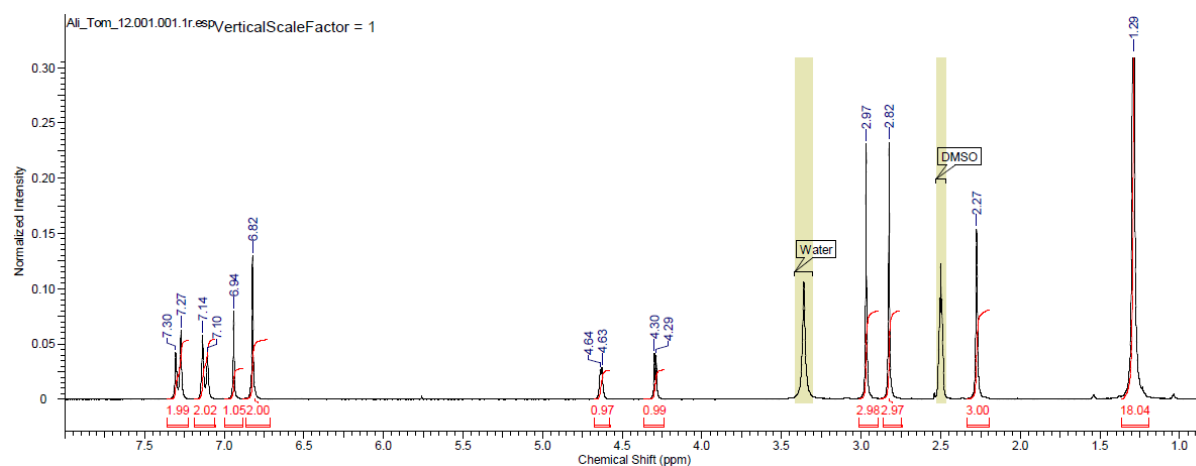
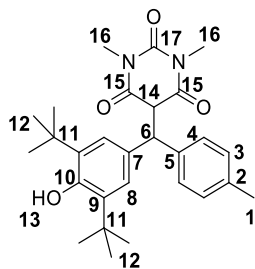
MB6c

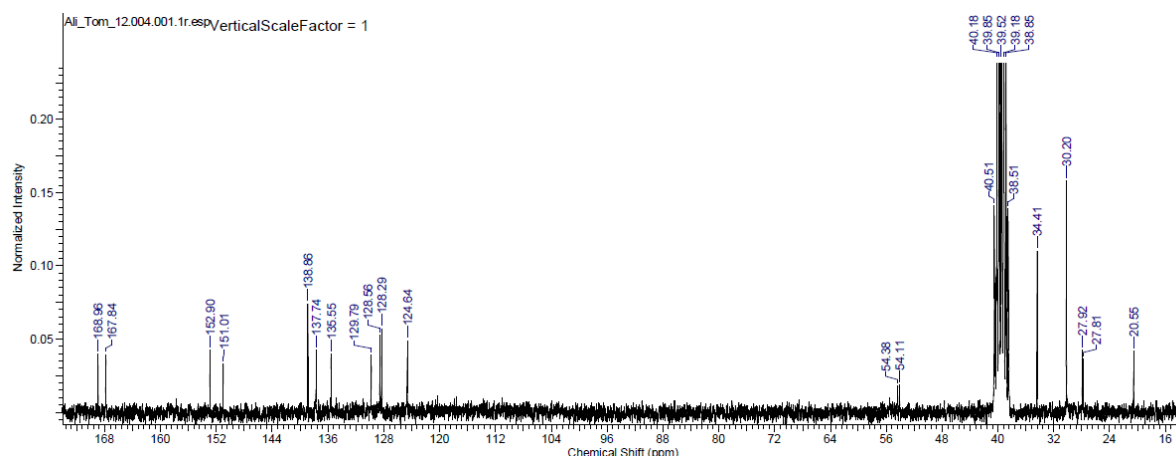


^1H NMR (d_6 -DMSO): δ 1.30 (s, 18H, $^{12}\text{CH}_3$), 2.20 (s, 3H, $^1\text{CH}_3$), 3.01 (s, 6H, $^{16}\text{CH}_3$), 5.34 (s, 1H, ^6CH), 6.42 (s, 1H, ^{13}OH), 6.88 (d, $^3J_{\text{HH}} = 7.75$ Hz, 2H, $^{3/4}\text{CH}$), 7.04 (d, $^3J_{\text{HH}} = 7.75$ Hz, 2H, $^{3/4}\text{CH}$), 7.14 (s, 2H, ^8CH)
 ^{13}C NMR (d_6 -DMSO): δ 20.7 ($^1\text{CH}_3$), 27.0 (^{11}C), 30.7 ($^{12}\text{CH}_3$), 34.4 ($^{16}\text{CH}_3$), 46.0 (^6CH), 88.9 (^{14}C), 125.6 (^8CH), 127.4, 137.1, 137.5, 144.7 ($^{2,5,7,9}\text{C}$), 128.6, 132.3 ($^{3,4}\text{CH}$), 150.8, 153.1 ($^{10,17}\text{CO}$), 161.8 (^{15}CO)



MB6c-H:





Quantum chemical calculations

1. Investigation setting

For the quantum chemical investigation of the ambident reactivity of **B** and **MB**, the (barbiturate)C(5)–C(electrophile) axis and the (barbiturate)O–C(electrophile) axis are chosen as reaction coordinates for C- and O-alkylation modeling, respectively. The solvent effects for DMSO are included by the COSMO solvation model with $\epsilon = 48$.

All reactions are modeled by performing relaxed scans along the relevant reaction coordinates. A step width of 0.02 Å is applied to carefully find the corresponding transition state structures. These structures are further utilized for single-point calculations. The identified minima structures from the relaxed scans are further optimized without constraints. Then, single-point calculations are performed using optimized molecular structures.

2. Relative energies and relative Gibbs energies

Table S3. Single-point relative energies and relative Gibbs energies for the optimized molecular and transition state structures for the alkylation of **B** and **MB** with **1a**, **2a,b**, **4a**, **5a-c** and **6a** at PW6B95-D3/TZVP/COSMO ($\epsilon = 48$) level of theory. The relative energies include ZPVE, which was scaled by a factor $f = 0.9914$. The relative Gibbs energies are calculated for a reaction temperature of 20 °C (293.15 K). The lowest dispersion complex is set to zero. All units are given in kJ/mol. (For further information see computational details.)

PW6B95-D3/def2-TZVPP/COSMO ($\epsilon = 48$)					
Nucleo- phile	Electro- phile	species	ΔE	ΔG	
B	1	a $\text{N}_\text{O}^\ominus + \text{E}^\oplus$	0.00	0.00	
		TS _O	3.68	6.67	
		N _O -E	-66.14	-68.21	
		N-E	-113.81	-112.93	
MB	1	a $\text{N}_\text{O}^\ominus + \text{E}^\oplus$	0.00	0.00	
		TS _O	1.97	3.47	
		N _O +E	-62.83	-66.28	
		N-E	-118.57	-117.83	
B	2	a $\text{N}^\ominus + \text{E}$	0.00	0.00	
		TS _C	21.39	24.96	
		N-E [⊖]	-23.45	-23.64	
		TS _{PT}	127.62	129.60	
		[⊖] N-E	-21.28	-23.40	
		N _O [⊖] +E	0.00	0.00	
		TS _O	40.92	42.62	

MB	2	a	$\text{N}_O\text{-E}^\ominus$	9.44	10.68
			$\text{N}^\ominus\text{+E}$	0.00	0.00
			TS_C	11.93	16.23
			$\text{N-E}^\ominus$	-39.37	-35.65
			TS_{PT}	128.84	128.90
			$^\ominus\text{N-E}$	-16.66	-18.31
			$\text{N}_O^\ominus\text{+E}$	0.00	0.00
			TS_O	41.90	42.55
		b	$\text{N}_O\text{-E}^\ominus$	16.16	16.48
			$\text{N}^\ominus\text{+E}$	0.00	0.00
			TS_C	18.22	24.24
			$\text{N-E}^\ominus$	-26.22	-21.67
			TS_{PT}	140.38	141.52
			$^\ominus\text{N-E}$	-5.29	-5.37
			$\text{N}_O^\ominus\text{+E}$	0.00	0.00
			TS_O	53.15	53.17
			$\text{N}_O\text{-E}^\ominus$	25.99	26.28
MB	4	a	$\text{N}^\ominus\text{+E}$	0.00	0.00
			TS_C	40.61	45.74
			$\text{N-E}^\ominus$	-7.52	-1.29
			TS_{PT}	160.57	161.57
			$^\ominus\text{N-E}$	24.92	28.60
			$\text{N}_O^\ominus\text{+E}$	0.00	0.00
			TS_O	68.21	68.59
			$\text{N}_O\text{-E}^\ominus$	49.91	49.21
B	5	a	$\text{N}^\ominus\text{+E}$	0.00	0.00
			TS_C	26.25	29.38
			$\text{N-E}^\ominus$	2.31	4.35
			TS_{PT}	118.44	121.79
			$^\ominus\text{N-E}$	-37.52	-36.77
			$\text{N}_O^\ominus\text{+E}$	0.00	0.00
			TS_O	40.52	42.37
			$\text{N}_O\text{-E}^\ominus$	28.97	30.97
MB	5	a	$\text{N}^\ominus\text{+E}$	0.00	0.00
			TS_C	21.51	24.06
			$\text{N-E}^\ominus$	-2.95	-2.18
			TS_{PT}	119.86	121.04
			$^\ominus\text{N-E}$	-30.65	-31.95
			$\text{N}_O^\ominus\text{+E}$	0.00	0.00
			TS_O	51.52	54.43
		b	$\text{N}_O\text{-E}^\ominus$	37.18	38.72
			$\text{N}^\ominus\text{+E}$	0.00	0.00
			TS_C	31.07	31.90
			$\text{N-E}^\ominus$	8.89	10.31
			TS_{PT}	143.04	143.89
			$^\ominus\text{N-E}$	-18.52	-19.14

			$\text{N}_\text{O}^\ominus + \text{E}$	0.00	0.00
			TS_O	65.12	65.14
			$\text{N}_\text{O}-\text{E}^\ominus$	51.67	48.13
	c		$\text{N}^\ominus + \text{E}$	0.00	0.00
			TS_C	42.19	44.71
			$\text{N}-\text{E}^\ominus$	23.72	24.41
			TS_PT	159.47	160.43
			$^\ominus\text{N}-\text{E}$	-2.13	-2.76
			$\text{N}_\text{O}^\ominus + \text{E}$	0.00	0.00
			TS_O	81.26	79.31
			$\text{N}_\text{O}-\text{E}^\ominus$	71.01	69.97
B	6	a	$\text{N}^\ominus + \text{E}$	0.00	0.00
			TS_C	41.91	44.26
			$\text{N}-\text{E}^\ominus$	-3.81	1.28
			TS_PT	-	-
			$^\ominus\text{N}-\text{E}$	-59.42	-57.79
			$\text{N}_\text{O}^\ominus + \text{E}$	0.00	0.00
			TS_O	67.19	68.86
			$\text{N}_\text{O}-\text{E}^\ominus$	41.63	38.86
MB	6	a	$\text{N}^\ominus + \text{E}$	0.00	0.00
			TS_C	32.66	39.48
			$\text{N}-\text{E}^\ominus$	-14.55	-9.01
			TS_PT	-	-
			$^\ominus\text{N}-\text{E}$	-51.66	-52.54
			$\text{N}_\text{O}^\ominus + \text{E}$	0.00	0.00
			TS_O	54.56	58.42
			$\text{N}_\text{O}-\text{E}^\ominus$	46.06	49.36
		b	$\text{N}^\ominus + \text{E}$	0.00	0.00
			TS_C	40.42	45.46
			$\text{N}-\text{E}^\ominus$	-0.19	6.16
			TS_PT	-	-
			$^\ominus\text{N}-\text{E}$	-34.78	-34.61
			$\text{N}_\text{O}^\ominus + \text{E}$	0.00	0.00
			TS_O	63.35	68.96
			$\text{N}_\text{O}-\text{E}^\ominus$	58.90	63.34

3. Obtained data from primarily performed quantum chemical calculations

Table S4. Energy values and ZPVE for the optimized molecular and transition state structures for the alkylation of **B** and **MB** with **1a**, **2a,b**, **4a**, **5a-c** and **6a** at BP86-D3/TZVP/COSMO ($\epsilon = 48$) level of theory (4th and 5th column). Single-point energies for PBE0-D3, PW6B95-D3, TPSS-D3 and TPSSH-D3 with def2-TZVPP basis and COSMO $\epsilon = 48$ (6th and 9th column). All units are given in Hartree.

Nucleo- phile	Electro- phile	species	BP86-D3		PBE0-D3		PW6B95-D3	TPSS-D3	TPSSH-D3
			<i>E</i>	<i>ZPVE</i>	<i>E</i>	<i>E</i>	<i>E</i>	<i>E</i>	<i>E</i>
B	1	a	$\text{N}_\text{O}^\ominus + \text{E}^\oplus$	-1070.567539	0.324109	-1069.287255	-1071.867653	-1070.714757	-1070.589302
			TS_O	-1070.565658	0.324422	-1069.287790	-1071.866561	-1070.713706	-1070.589048

MB	1	a	N _O -E	-1070.582001	0.326289	-1069.319256	-1071.895006	-1070.733294	-1070.612749
			N-E	-1070.605312	0.326972	-1069.339527	-1071.913838	-1070.750028	-1070.630130
			N _O [⊖] +E [⊕]	-1149.211169	0.378232	-1147.827504	-1150.608666	-1149.374671	-1149.241351
			TS _O	-1149.208917	0.378596	-1147.830211	-1150.608275	-1149.374326	-1149.242458
			N _O +E	-1149.222768	0.380354	-1147.859272	-1150.634700	-1149.392156	-1149.264175
			N-E	-1149.250028	0.381165	-1147.881991	-1150.656736	-1149.411911	-1149.284437
B	2	a	N [⊖] +E	-1293.769931	0.296532	-1292.260880	-1295.277355	-1293.912799	-1293.756741
			TS _C	-1293.766511	0.296954	-1292.257098	-1295.269625	-1293.907449	-1293.751522
			N-E [⊖]	-1293.779791	0.299032	-1292.279188	-1295.288764	-1293.919691	-1293.767028
			TS _{PT}	-1293.721219	0.292090	-1292.216948	-1295.224343	-1293.859080	-1293.703983
			[⊖] N-E	-1293.778470	0.298585	-1292.279251	-1295.287495	-1293.919628	-1293.766877
			N _O [⊖] +E	-1293.765883	0.296359	-1292.258777	-1295.275118	-1293.909349	-1293.753699
			TS _O	-1293.751234	0.296577	-1292.246768	-1295.259750	-1293.896492	-1293.741279
			N _O -E [⊖]	-1293.758286	0.298195	-1292.261003	-1295.273344	-1293.904402	-1293.751360
MB	2	a	N [⊖] +E	-1372.412997	0.350916	-1370.801103	-1374.016324	-1372.572237	-1372.408476
			TS _C	-1372.411344	0.351188	-1370.798922	-1374.012050	-1372.569019	-1372.405339
			N-E [⊖]	-1372.424587	0.353270	-1370.821737	-1374.033655	-1372.580985	-1372.421008
			TS _{PT}	-1372.360509	0.345889	-1370.755187	-1373.962267	-1372.516275	-1372.353673
			[⊖] N-E	-1372.416882	0.352464	-1370.816416	-1374.024204	-1372.575692	-1372.415423
			N _O [⊖] +E	-1372.409214	0.350514	-1370.799898	-1374.017121	-1372.569239	-1372.406095
			TS _O	-1372.393887	0.350575	-1370.787164	-1374.001224	-1372.556041	-1372.393386
			N _O -E [⊖]	-1372.399723	0.352484	-1370.800541	-1374.012920	-1372.563087	-1372.402509
	2	b	N [⊖] +E	-1486.996843	0.382126	-1485.254759	-1488.727786	-1487.169400	-1486.992029
			TS _C	-1486.993176	0.382583	-1485.250865	-1488.721300	-1487.163579	-1486.986527
			N-E [⊖]	-1487.003846	0.384441	-1485.270578	-1488.740066	-1487.173283	-1486.999720
			TS _{PT}	-1486.939919	0.377095	-1485.204350	-1488.669329	-1487.108879	-1486.932724
			[⊖] N-E	-1486.996546	0.383707	-1485.265818	-1488.731370	-1487.168650	-1486.994759
			N _O [⊖] +E	-1486.992905	0.381931	-1485.253297	-1488.727938	-1487.166276	-1486.989429
			TS _O	-1486.973478	0.382091	-1485.237466	-1488.707852	-1487.149529	-1486.973179
			N _O -E [⊖]	-1486.979438	0.383727	-1485.249790	-1488.719821	-1487.155912	-1486.981716
MB	4	a	N [⊖] +E	-1540.775593	0.428880	-1538.955039	-1542.586909	-1540.959259	-1540.776535
			TS _C	-1540.764532	0.429312	-1538.945556	-1542.571868	-1540.946650	-1540.764512
			N-E [⊖]	-1540.776447	0.431072	-1538.965024	-1542.591948	-1540.957396	-1540.778381
			TS _{PT}	-1540.712505	0.423988	-1538.899629	-1542.520899	-1540.893730	-1540.712197
			[⊖] N-E	-1540.772050	0.431129	-1538.955056	-1542.579646	-1540.947567	-1540.768407
			N _O [⊖] +E	-1540.775422	0.429089	-1538.956255	-1542.587992	-1540.959592	-1540.777119
			TS _O	-1540.746517	0.428813	-1538.934511	-1542.561737	-1540.935023	-1540.753731
			N _O -E [⊖]	-1540.749951	0.430270	-1538.943604	-1542.570154	-1540.939200	-1540.759652
B	5	a	N [⊖] +E	-984.220143	0.204971	-983.049096	-985.395185	-984.338564	-984.214613
			TS _C	-984.215038	0.205570	-983.044343	-985.385780	-984.331225	-984.207536
			N-E [⊖]	-984.221360	0.207612	-983.057974	-985.396923	-984.336465	-984.215490

MB	5	a	TS _{PT}	-984.175818	0.201444	-983.009727	-985.346576	-984.288811	-984.166165
			[⊖] N-E	-984.231260	0.206997	-983.072004	-985.411485	-984.347869	-984.228198
			N _O [⊖] +E	-984.216137	0.204641	-983.045671	-985.391383	-984.335153	-984.211208
			TS _O	-984.199973	0.205024	-983.034005	-985.376329	-984.321294	-984.197925
			N _O -E [⊖]	-984.201634	0.206493	-983.041357	-985.382185	-984.323123	-984.201686
			N [⊖] +E	-1062.863156	0.259175	-1061.589673	-1064.135391	-1062.998247	-1062.866622
		b	TS _C	-1062.859236	0.259705	-1061.586339	-1064.127724	-1062.992401	-1062.861125
			N-E [⊖]	-1062.865497	0.261725	-1061.600310	-1064.139045	-1062.997841	-1062.869377
			TS _{PT}	-1062.816162	0.255240	-1061.549252	-1064.085839	-1062.947184	-1062.817103
			[⊖] N-E	-1062.869836	0.260797	-1061.609561	-1064.148673	-1063.004328	-1062.877134
			N _O [⊖] +E	-1062.858579	0.258831	-1061.586858	-1064.133679	-1062.994643	-1062.863392
			TS _O	-1062.839650	0.259365	-1061.573237	-1064.114587	-1062.978367	-1062.847915
	6	a	N _O -E [⊖]	-1062.841837	0.260626	-1061.580914	-1064.121297	-1062.981406	-1062.852577
			N [⊖] +E	-1177.447213	0.290521	-1176.043466	-1178.847443	-1177.595496	-1177.450268
			TS _C	-1177.440411	0.291188	-1176.037495	-1178.836271	-1177.586444	-1177.441719
			N-E [⊖]	-1177.445880	0.293098	-1176.050128	-1178.846612	-1177.591241	-1177.449142
			TS _{PT}	-1177.392256	0.286812	-1175.995040	-1178.789285	-1177.536721	-1177.392946
			[⊖] N-E	-1177.449941	0.292053	-1176.059297	-1178.856015	-1177.597535	-1177.456742
		b	N _O [⊖] +E	-1177.446312	0.290750	-1176.042941	-1178.847304	-1177.594611	-1177.449452
			TS _O	-1177.420301	0.290817	-1176.023724	-1178.822566	-1177.571918	-1177.428009
			N _O -E [⊖]	-1177.421858	0.291696	-1176.030448	-1178.828562	-1177.574608	-1177.432117
			N [⊖] +E	-1196.902856	0.330141	-1195.465246	-1198.335693	-1197.056900	-1196.911407
			TS _C	-1196.891575	0.330677	-1195.455939	-1198.320156	-1197.043744	-1196.899043
			N-E [⊖]	-1196.895693	0.332399	-1195.466642	-1198.328898	-1197.047308	-1196.905042
B	6	a	TS _{PT}	-1196.841679	0.326255	-1195.411426	-1198.271103	-1196.992552	-1196.848644
			[⊖] N-E	-1196.899242	0.331406	-1195.475574	-1198.337757	-1197.053284	-1196.912348
			N _O [⊖] +E	-1196.903358	0.330102	-1195.466607	-1198.336739	-1197.057952	-1196.912569
			TS _O	-1196.870127	0.329812	-1195.440594	-1198.305500	-1197.029233	-1196.884815
			N _O -E [⊖]	-1196.871680	0.331162	-1195.447072	-1198.310745	-1197.030850	-1196.888168
			N [⊖] +E	-1643.608878	0.450885	-1641.654590	-1645.619237	-1643.833763	-1643.641261
		b	TS _C	-1643.599221	0.451152	-1641.643990	-1645.603538	-1643.821439	-1643.628942
			N-E [⊖]	-1643.610791	0.453107	-1641.665364	-1645.622891	-1643.831696	-1643.643023
			TS _{PT}	-	-	-	-	-	-
			[⊖] N-E	-1643.625366	0.453377	-1641.686846	-1645.644338	-1643.848611	-1643.661292
			N _O [⊖] +E	-1643.608967	0.450933	-1641.654148	-1645.619175	-1643.833431	-1643.640896
			TS _O	-1643.583697	0.450689	-1641.633905	-1645.593343	-1643.809405	-1643.618158
	6	a	N _O -E [⊖]	-1643.586197	0.452041	-1641.645069	-1645.604416	-1643.814997	-1643.625695
			N [⊖] +E	-1722.251075	0.505278	-1720.194496	-1724.359183	-1722.492494	-1722.292536
			TS _C	-1722.245230	0.505633	-1720.187046	-1724.347095	-1722.483973	-1722.283815
			N-E [⊖]	-1722.257334	0.507549	-1720.209184	-1724.366976	-1722.494703	-1722.298438
			TS _{PT}	-	-	-	-	-	-
			[⊖] N-E	-1722.263023	0.507049	-1720.223288	-1724.380617	-1722.503942	-1722.309102

		$\text{N}_\text{O}^\ominus + \text{E}$	-1722.249866	0.505245	-1720.193255	-1724.357762	-1722.491696	-1722.291542
		TS_O	-1722.229630	0.505175	-1720.176977	-1724.336912	-1722.472128	-1722.273094
		$\text{N}_\text{O}-\text{E}^\ominus$	-1722.230358	0.506327	-1720.182126	-1724.341290	-1722.473017	-1722.275545
b		$\text{N}^\ominus + \text{E}$	-1741.706315	0.544763	-1739.616076	-1743.846256	-1741.954278	-1741.753814
		TS_C	-1741.706638	0.546989	-1739.625313	-1743.848537	-1741.950286	-1741.753897
		$\text{N}-\text{E}^\ominus$	-1741.696032	0.544767	-1739.605634	-1743.830866	-1741.941072	-1741.741016
		TS_PT	-	-	-	-	-	-
		$^\ominus\text{N}-\text{E}$	-1741.711377	0.546533	-1739.638385	-1743.861260	-1741.958320	-1741.763378
		$\text{N}_\text{O}^\ominus + \text{E}$	-1741.705740	0.544489	-1739.614951	-1743.844507	-1741.953376	-1741.752730
		TS_O	-1741.679853	0.544653	-1739.595216	-1743.820541	-1741.928868	-1741.730047
		$\text{N}_\text{O}-\text{E}^\ominus$	-1741.680048	0.545555	-1739.598341	-1743.823131	-1741.929152	-1741.731383

Table S5. Calculated values for chemical potential (μ), energy (E), entropy (S) and enthalpy (H) and ZPVE for the optimized molecular and transition state structures for the alkylation of **B** and **MB** with **1a**, **2a,b**, **4a**, **5a-c** and **6a** at BP86-D3/TZVP/COSMO ($\epsilon = 48$) level of theory. ZPVE was scaled by a factor $f = 0.9914$. All values are calculated for a reaction temperature of 20 °C (293.15 K). (For further information see computational details.)

BP86-D3/TZVP/COSMO ($\epsilon = 48$)								
Nucleo- phile	Electro- phile	species	μ [kJ/mol]	E [kJ/mol]	S [kJ/mol/K]	H [kJ/mol]	$ZPVE$ [kJ/mol]	
B	1	a	$\text{N}_\text{O}^\ominus + \text{E}^\oplus$	708.1300	901.3600	0.6675	903.8000	843.6000
			TS_O	711.9300	899.7100	0.6489	902.1500	844.4000
			$\text{N}_\text{O}-\text{E}$	711.7300	905.5100	0.6694	907.9500	849.3000
			$\text{N}-\text{E}$	716.4600	906.8400	0.6578	909.2800	851.1000
MB	1	a	$\text{N}_\text{O}^\ominus + \text{E}^\oplus$	840.9600	1050.2000	0.7221	1052.6400	984.5000
			TS_O	843.4000	1048.8600	0.7092	1051.2900	985.4000
			$\text{N}_\text{O} + \text{E}$	843.0300	1054.5100	0.7297	1056.9500	990.0000
			$\text{N}-\text{E}$	849.3400	1055.9400	0.7131	1058.3800	992.1000
B	2	a	$\text{N}^\ominus + \text{E}$	635.4800	832.4700	0.6803	834.9000	771.8000
			TS_C	640.1500	831.0200	0.6594	833.4500	772.9000
			$\text{N}-\text{E}^\ominus$	641.7900	836.9900	0.6742	839.4200	778.3000
			TS_PT	625.9000	818.7400	0.6662	821.1800	760.3000
			$^\ominus\text{N}-\text{E}$	638.7000	836.4400	0.6829	838.8800	777.2000
			$\text{N}_\text{O}^\ominus + \text{E}$	633.3100	832.3500	0.6873	834.7900	771.4000
			TS_O	635.5800	830.3100	0.6726	832.7500	772.0000
			$\text{N}_\text{O}-\text{E}^\ominus$	639.3300	834.9800	0.6757	837.4200	776.2000
MB	2	a	$\text{N}^\ominus + \text{E}$	768.9900	981.7400	0.7340	984.1700	913.4000
			TS_C	774.0000	980.0400	0.7112	982.4800	914.1000
			$\text{N}-\text{E}^\ominus$	778.8400	985.7100	0.7140	988.1500	919.5000
			TS_PT	755.9600	967.2800	0.7292	969.7200	900.3000
			$^\ominus\text{N}-\text{E}$	771.3700	984.9000	0.7367	987.3400	917.4000
			$\text{N}_\text{O}^\ominus + \text{E}$	766.9400	981.0500	0.7387	983.4900	912.4000
			TS_O	767.7500	979.0000	0.7289	981.4300	912.5000
			$\text{N}_\text{O}-\text{E}^\ominus$	772.3900	984.2100	0.7309	986.6400	917.5000
	2	b	$\text{N}^\ominus + \text{E}$	839.7900	1070.1900	0.7943	1072.6300	994.6000

			TS _C	847.0000	1068.5700	0.7642	1071.0100	995.8000
			N-E [⊖]	850.3600	1073.9200	0.7709	1076.3600	1001.0000
			TS _{PT}	827.8300	1055.5000	0.7849	1057.9300	981.5000
			[⊖] N-E	843.8300	1073.1300	0.7905	1075.5700	998.7000
			No [⊖] +E	840.2200	1069.6000	0.7908	1072.0300	994.1000
			TS _O	840.6500	1067.8300	0.7833	1070.2700	994.5000
			No-E [⊖]	845.1900	1072.4000	0.7834	1074.8400	998.8000
MB	4	a	N [⊖] +E	951.3300	1199.6500	0.8554	1202.0900	1116.0000
			TS _C	957.5800	1197.8400	0.8279	1200.2800	1117.0000
			N-E [⊖]	963.2700	1202.4500	0.8242	1204.8800	1122.0000
			TS _{PT}	939.5900	1184.9300	0.8452	1187.3700	1104.0000
			[⊖] N-E	960.8600	1203.0100	0.8344	1205.4500	1122.0000
			No [⊖] +E	953.6800	1199.7600	0.8477	1202.2000	1117.0000
			TS _O	953.3400	1196.8000	0.8388	1199.2400	1116.0000
			No-E [⊖]	956.0600	1201.1500	0.8444	1203.5900	1120.0000
B	5	a	N [⊖] +E	409.7600	582.1100	0.5962	584.5400	533.5000
			TS _C	414.4500	581.0600	0.5767	583.5000	535.1000
			N-E [⊖]	418.6700	586.5500	0.5810	588.9800	540.4000
			TS _{PT}	403.9300	570.1300	0.5753	572.5700	524.3000
			[⊖] N-E	415.7800	585.4100	0.5870	587.8500	538.8000
			No [⊖] +E	405.9600	581.8200	0.6082	584.2500	532.7000
			TS _O	408.8100	580.1200	0.5927	582.5600	533.7000
			No-E [⊖]	412.7800	584.3800	0.5937	586.8200	537.5000
MB	5	a	N [⊖] +E	542.7100	731.0400	0.6508	733.4800	674.6000
			TS _C	546.6400	730.0100	0.6338	732.4400	676.0000
			N-E [⊖]	550.1200	738.0900	0.6412	735.6500	681.2000
			TS _{PT}	533.6500	718.7000	0.6396	721.1400	664.4000
			[⊖] N-E	545.6300	733.8300	0.6503	736.2700	678.8000
			No [⊖] +E	537.7400	730.7300	0.6667	733.1700	673.7000
			TS _O	542.0400	729.4700	0.6477	731.9000	675.1000
			No-E [⊖]	543.9500	733.5400	0.6550	735.9800	678.4000
		b	N [⊖] +E	615.7800	819.5000	0.7033	821.9400	756.2000
			TS _C	618.3500	818.6900	0.6917	821.1200	757.9000
			N-E [⊖]	623.9100	823.9800	0.6908	826.4100	762.9000
			TS _{PT}	606.9800	807.6400	0.6928	810.0800	746.5000
			[⊖] N-E	619.1500	821.9500	0.7001	824.3900	760.2000
			No [⊖] +E	616.4300	819.7600	0.7019	822.1900	756.8000
			TS _O	616.6200	817.9000	0.6949	820.3300	757.0000
			No-E [⊖]	615.3500	821.4500	0.7114	823.8800	759.3000
		c	N [⊖] +E	713.5300	927.3700	0.7378	929.8100	859.3000
			TS _C	717.4500	925.9400	0.7195	928.3800	860.7000
			N-E [⊖]	720.1000	930.8100	0.7271	933.2500	865.2000

			TS _{PT}	704.3800	914.7800	0.7260	917.2100	849.2000
			[⊖] N-E	716.1900	928.9300	0.7340	931.3700	862.6000
			N _O [⊖] +E	711.7500	927.1500	0.7431	929.5900	859.2000
			TS _O	709.0400	924.6400	0.7438	927.0800	858.5000
			N _O -E [⊖]	713.4700	928.5800	0.7421	931.0200	862.0000
B	6	a	N [⊖] +E	1004.7200	1256.6600	0.8677	1259.0900	1174.0000
			TS _C	1007.7600	1254.5000	0.8500	1256.9400	1174.0000
			N-E [⊖]	1015.5900	1259.4900	0.8403	1261.9200	1179.0000
			TS _{PT}	-	-	-	-	-
			[⊖] N-E	1012.8300	1260.9000	0.8546	1263.3400	1180.0000
			N _O [⊖] +E	1006.3300	1256.6600	0.8622	1259.1000	1174.0000
			TS _O	1007.3700	1253.1300	0.8467	1255.5700	1173.0000
			N _O -E [⊖]	1006.4400	1257.5900	0.8651	1260.0300	1177.0000
MB	6	a	N [⊖] +E	1138.9900	1406.0100	0.9192	1408.4500	1315.0000
			TS _C	1146.7300	1403.8100	0.8853	1406.2500	1316.0000
			N-E [⊖]	1150.4400	1409.0800	0.8906	1411.5200	1321.0000
			TS _{PT}	-	-	-	-	-
			[⊖] N-E	1142.7200	1409.0400	0.9168	1411.4800	1320.0000
			N _O [⊖] +E	1139.1600	1405.6100	0.9173	1408.0500	1315.0000
			TS _O	1142.8400	1402.6400	0.8946	1405.0800	1315.0000
			N _O -E [⊖]	1145.2700	1406.2600	0.8986	1408.7000	1318.0000
		b	N [⊖] +E	1235.6600	1513.5900	0.9564	1516.0200	1418.0000
			TS _C	1240.7100	1510.7800	0.9296	1513.2100	1418.0000
			N-E [⊖]	1247.8100	1516.1800	0.9238	1518.6200	1424.0000
			TS _{PT}	-	-	-	-	-
			[⊖] N-E	1240.4400	1516.1500	0.9488	1518.5900	1423.0000
			N _O [⊖] +E	1234.3100	1513.1600	0.9595	1515.5900	1417.0000
			TS _O	1240.3500	1509.8600	0.9277	1512.3000	1418.0000
			N _O -E [⊖]	1241.5300	1513.1000	0.9347	1515.5400	1420.0000

4. Cartesian coordinates of optimized molecular and transition state structures

B + 1a									
N _O [⊖] +E [⊖]				TS _O			N _O -E		
C	0.9464663	-1.7844871	1.6040991	C	1.1402708	-1.8195720	1.5374208	C	-3.0275415 -0.0757135 -1.4318767
C	0.8737729	-0.4976938	1.0854366	C	0.9539355	-0.5647253	0.9653413	C	-1.6764264 0.0601282 -1.1022631
C	1.6030230	-0.1498146	-0.0885113	C	1.5705992	-0.2371170	-0.2673752	C	-1.2991412 0.4388904 0.1924452
C	2.3902281	-1.1670069	-0.7074186	C	2.3927155	-1.2137061	-0.8804838	C	-2.2957439 0.6742759 1.1490519
C	2.4602479	-2.4391010	-0.1742518	C	2.5834270	-2.4575175	-0.2938492	C	-3.6448081 0.5427762 0.8123340
C	1.7186486	-2.7807844	0.9815874	C	1.9366719	-2.7946157	0.9125281	C	-4.0357783 0.1632702 -0.4834221
H	0.3587717	-2.0381861	2.4875579	H	0.6317888	-2.0614682	2.4724831	H	-3.3036421 -0.3724900 -2.4463869
H	0.2213439	0.2260661	1.5637243	H	0.2829788	0.1423433	1.4469036	H	-0.9109767 -0.1364135 -1.8546278
H	2.9371094	-0.9265015	-1.6211018	H	2.8630120	-0.9861839	-1.8394396	H	-2.0152339 0.9639970 2.1645924

H	3.0664970	-3.2020835	-0.6654518	H	3.2159914	-3.1970365	-0.7886093	H	-4.4079918	0.7320750	1.5707879
C	1.4656278	1.0860483	-0.7723310	C	1.2195987	0.9426320	-1.0289213	C	0.1502707	0.6412948	0.5767578
C	0.9339849	2.3329541	-0.3175147	C	0.8013606	2.2259395	-0.4707599	C	0.6790095	2.0416249	0.3584465
C	0.5804377	3.2958491	-1.3025575	C	0.2264605	3.1872648	-1.3353500	C	0.2672561	2.8292239	-0.7260135
C	0.7662732	2.6876090	1.0467489	C	1.0104530	2.5868424	0.8765563	C	1.6386020	2.5561852	1.2424416
C	0.0293250	4.5147229	-0.9433871	C	-0.1654891	4.4305993	-0.8592708	C	0.8098623	4.1009030	-0.9218433
H	0.7145697	3.0452006	-2.3557436	H	0.0623785	2.9260259	-2.3812918	H	-0.4851565	2.4506837	-1.4196259
C	0.2315164	3.9204820	1.3958347	C	0.6291680	3.8454971	1.3427858	C	2.1734954	3.8318133	1.0472565
H	1.1155774	2.0213537	1.8335239	H	1.5214545	1.9047511	1.5545921	H	1.9700214	1.9528634	2.0909459
C	-0.1662652	4.8496894	0.4138379	C	0.0202698	4.7832291	0.4941048	C	1.7685091	4.6271838	-0.0380910
H	-0.2531054	5.2303065	-1.7179614	H	-0.6214781	5.1502341	-1.5427313	H	0.4800082	4.6993963	-1.7742088
H	0.1308455	4.1811784	2.4510052	H	0.8161910	4.1061799	2.3865090	H	2.9179011	4.2162381	1.7482741
H	1.8778220	1.1002374	-1.7837085	H	1.6844602	1.0013375	-2.0146837	H	0.2953764	0.3731332	1.6350957
C	1.6941169	-4.1939074	1.4779801	C	2.0370490	-4.1825426	1.4784105	C	-5.4921500	-0.0191633	-0.8323653
H	1.4193280	-4.2505426	2.5393704	H	1.9350730	-4.1837445	2.5721379	H	-5.6716954	0.1426870	-1.9042628
H	0.9352536	-4.7523221	0.9024073	H	1.2185814	-4.7979179	1.0684358	H	-5.8227303	-1.0431957	-0.5941088
H	2.6586938	-4.6964270	1.3226939	H	2.9845637	-4.6664335	1.2056320	H	-6.1308404	0.6710084	-0.2635086
C	-0.7891354	6.1602909	0.7974669	C	-0.4302125	6.1253758	1.0038391	C	2.3176655	6.0185249	-0.2302694
H	-0.5029747	6.4642634	1.8129787	H	0.0029988	6.3522713	1.9867642	H	3.3205135	6.1191342	0.2071227
H	-0.5162569	6.9574847	0.0922156	H	-0.1578417	6.9289325	0.3040973	H	2.3717608	6.2849662	-1.2951218
H	-1.8884424	6.0712615	0.7764676	H	-1.5274107	6.1466026	1.1062605	H	1.6680098	6.7613794	0.2604446
O	-0.5840482	0.3713774	-2.0815015	O	-0.4453640	0.3444701	-1.9617102	O	1.0419433	-0.2389850	-0.2200302
C	-1.0835902	-0.5031601	-1.3183987	C	-1.0987205	-0.4851052	-1.2078397	C	1.0245085	-1.5554264	0.0302907
N	-0.7419732	-1.8560635	-1.5603164	N	-0.8167462	-1.8440546	-1.3912738	N	1.9144734	-2.2232162	-0.7833241
C	-1.9069977	-0.2601452	-0.2038456	C	-1.9931098	-0.1286351	-0.2112218	C	0.2653512	-2.2350938	0.9483281
C	-1.1041325	-2.9347751	-0.7825875	C	-1.2859866	-2.8692481	-0.5902685	C	2.1211369	-3.5960318	-0.7465746
C	-2.3552659	-1.3081794	0.6485681	C	-2.5752086	-1.1156170	0.6485311	C	0.4001363	-3.6614907	1.0667453
H	-2.1747889	0.7656655	0.0350517	H	-2.2102371	0.9218143	-0.0397812	H	-0.4671161	-1.7372887	1.5737315
N	-1.9244888	-2.6071982	0.2805521	N	-2.1712922	-2.4454204	0.3849704	N	1.3413379	-4.2471261	0.1888047
O	-0.7310938	-4.0937102	-1.0144064	O	-0.9485955	-4.0486117	-0.7367199	O	2.9280631	-4.1642461	-1.4848368
O	-3.0584696	-1.1847057	1.6767598	O	-3.3617792	-0.9001429	1.5913139	O	-0.2304838	-4.3878412	1.8523988
H	-0.1048857	-2.0423413	-2.3327118	H	-0.1122790	-2.0887388	-2.0852378	H	1.4596592	-5.2587742	0.2477168
H	-2.2136666	-3.3775703	0.8818346	H	-2.5519951	-3.1708363	0.9922969	H	2.4735321	-1.6880773	-1.4469677

B + 1a

N-E

C	0.9464663	-1.7844871	1.6040991
C	-1.0713699	-0.9544712	-2.6226812
C	-0.2127631	-0.6651952	-1.5612371
C	-0.3796865	0.5042979	-0.8034123
C	-1.4188594	1.3797095	-1.1481975
C	-2.2778991	1.0874729	-2.2118981
C	-2.1221629	-0.0857724	-2.9664129
H	-0.9266446	-1.8743900	-3.1944004
H	0.5946875	-1.3557430	-1.3106628
H	-1.5618823	2.3003334	-0.5770983
H	-3.0830176	1.7836130	-2.4582924
C	0.4853951	0.7822827	0.4190740

C	1.9509321	0.4137997	0.2114880
C	2.6215804	1.0509018	-0.8510753
C	2.6821132	-0.4718472	1.0089096
C	3.9701606	0.8084577	-1.1025046
H	2.0717338	1.7457978	-1.4902725
C	4.0394998	-0.7151059	0.7526298
H	2.2016007	-1.0078085	1.8260650
C	4.7092225	-0.0842262	-0.3029111
H	4.4621405	1.3221988	-1.9322663
H	4.5822796	-1.4160022	1.3915553
H	0.4678013	1.8689476	0.6012276
C	-3.0296495	-0.3900907	-4.1326721
H	-3.2054840	-1.4706563	-4.2321577
H	-4.0010950	0.1124568	-4.0278536
H	-2.5790348	-0.0445781	-5.0772831
C	6.1675442	-0.3479118	-0.5871936
H	6.6060373	-1.0264998	0.1568423
H	6.3000560	-0.8024754	-1.5814485
H	6.7480205	0.5874345	-0.5814293
C	-0.1881645	0.1694380	1.7175248
C	-1.2789979	1.1320015	2.1586898
C	-0.6506199	-1.2564420	1.4749698
N	-2.5802688	0.7570160	1.8820523
O	-1.0270413	2.2167597	2.6746654
N	-2.0043970	-1.4175907	1.2194294
O	0.1083797	-2.2185283	1.4462128
C	-3.0054248	-0.4673191	1.3736742
O	-4.1808804	-0.6991033	1.1205930
H	0.5580879	0.1557845	2.5224563
H	-3.3194259	1.4312044	2.0877065
H	-2.3192953	-2.3504476	0.9484265

MB + 1a											
N _O [⊖] +E [⊕]				TS _O				N _O -E			
C	-1.1927883	-1.6601782	-1.5819435	C	-1.3751858	-1.5820272	-1.5366399	C	-3.1456822	0.2938125	-1.3223099
C	-1.0505377	-0.3985792	-1.0340426	C	-1.0708662	-0.3631701	-0.9411752	C	-1.7859986	0.3600479	-1.0063442
C	-1.6918666	-0.0596851	0.1929736	C	-1.6663827	0.0129292	0.2854820	C	-1.3764979	0.7132478	0.2854456
C	-2.4190433	-1.0907998	0.8568755	C	-2.5738264	-0.8900875	0.8815490	C	-2.3501746	0.9890168	1.2547863
C	-2.5767445	-2.3445225	0.2837551	C	-2.8883161	-2.1005856	0.2703975	C	-3.7076771	0.9264193	0.9321890
C	-1.9604723	-2.6588305	-0.9410969	C	-2.2772560	-2.4800853	-0.9372759	C	-4.1308608	0.5817201	-0.3632613
H	-0.6747155	-1.9017477	-2.5116869	H	-0.8835898	-1.8580752	-2.4716005	H	-3.4466337	0.0079423	-2.3328891
H	-0.3983400	0.3202047	-1.5257907	H	-0.3312930	0.2835188	-1.4104121	H	-1.0404426	0.1186309	-1.7656168
H	-2.8802407	-0.8712231	1.8213250	H	-3.0241966	-0.6346038	1.8428949	H	-2.0450573	1.2505615	2.2709061
H	-3.1512416	-3.1097426	0.8077802	H	-3.5925941	-2.7806629	0.7535825	H	-4.4524968	1.1392983	1.7025824
C	-1.5398219	1.1866928	0.8523444	C	-1.2286100	1.1704043	1.0515067	C	0.0879378	0.8432443	0.6560929
C	-1.0572481	2.4300470	0.3308957	C	-0.8046178	2.4505291	0.4694063	C	0.6389949	2.2389679	0.4687193
C	-1.0285718	2.7617217	-1.0484119	C	-1.0142814	2.7953334	-0.8794370	C	0.5024669	2.9138595	-0.7542175

C	-0.5797891	3.3968659	1.2564842	C	-0.1947866	3.4063094	1.3130086	C	1.3097355	2.8729604	1.5211829
C	-0.4910896	3.9695542	-1.4743354	C	-0.5891652	4.0305574	-1.3721532	C	1.0335172	4.1930192	-0.9169704
H	-1.4810486	2.0941972	-1.7802598	H	-1.5465895	2.1154939	-1.5434388	H	-0.0211296	2.4355625	-1.5835816
C	-0.0271922	4.5898472	0.8185165	C	0.2390096	4.6272764	0.8117732	C	1.8281670	4.1624314	1.3584502
H	-0.6031617	3.1615177	2.3211505	H	-0.0328771	3.1602745	2.3633307	H	1.4297384	2.3565385	2.4763674
C	0.0416892	4.8966186	-0.5571165	C	0.0602999	4.9608749	-0.5462139	C	1.7003392	4.8440609	0.1384335
H	-0.4942634	4.2112104	-2.5389000	H	-0.7724056	4.2774964	-2.4200542	H	0.9257659	4.7015297	-1.8779595
H	0.3597449	5.3052566	1.5468672	H	0.7231416	5.3424270	1.4805936	H	2.3457649	4.6424037	2.1921142
H	-1.8851946	1.2118590	1.8875556	H	-1.7145263	1.2629503	2.0249575	H	0.2361331	0.5436424	1.7054254
C	-2.0357531	-4.0419933	-1.5140086	C	-2.5241607	-3.8363849	-1.5384229	C	-5.5972204	0.5426278	-0.7161350
H	-1.9746106	-4.0315348	-2.6106357	H	-2.4323607	-3.8174347	-2.6330328	H	-5.7925985	-0.1489180	-1.5473500
H	-1.1804181	-4.6256261	-1.1351171	H	-1.7749064	-4.5490799	-1.1560575	H	-6.2091969	0.2357469	0.1436977
H	-2.9529752	-4.5607557	-1.2052761	H	-3.5159448	-4.2249412	-1.2705603	H	-5.9476576	1.5399905	-1.0279311
C	0.6728671	6.1754247	-1.0276061	C	0.5598711	6.2748029	-1.0858370	C	2.2344257	6.2438701	-0.0359809
H	1.7639141	6.0427012	-1.1209302	H	1.6549414	6.2481345	-1.2074431	H	2.6896492	6.3772669	-1.0279144
H	0.2929863	6.4770017	-2.0127478	H	0.1199091	6.5037459	-2.0654696	H	1.4213681	6.9827133	0.0499570
H	0.5068252	6.9933187	-0.3128236	H	0.3330114	7.1012856	-0.3967035	H	2.9857322	6.4865561	0.7276782
O	0.5120231	0.5452960	2.2473966	O	0.3755217	0.5717401	1.9202727	O	0.9300350	-0.0275380	-0.1848659
C	0.8940501	-0.4500760	1.5676428	C	0.8523137	-0.5034449	1.3509705	C	0.8709816	-1.3554460	-0.0011135
N	1.7273449	-0.2259588	0.4339424	N	1.7620637	-0.3363274	0.2938368	N	1.6908624	-2.0247937	-0.8878328
C	0.4923265	-1.7729653	1.8000542	C	0.4504738	-1.7781792	1.6898161	C	0.1212045	-2.0252828	0.9298393
C	2.0755445	-1.2251542	-0.4632242	C	2.1738927	-1.4003523	-0.5042034	C	1.7972094	-3.4229122	-0.8713319
C	0.7909420	-2.8431681	0.9191433	C	0.8260652	-2.9265437	0.9275350	C	0.1682909	-3.4524806	1.0134810
H	-0.1618873	-1.9711271	2.6443575	H	-0.2745605	-1.9043983	2.4880126	N	1.0337431	-4.0881977	0.0791910
N	1.6242921	-2.5105003	-0.1899268	N	1.6937271	-2.6615631	-0.1682098	O	2.5293496	-4.0307048	-1.6583284
O	2.7438681	-0.9771585	-1.4799988	O	2.9193876	-1.2252257	-1.4774155	O	-0.4847867	-4.1318437	1.8262628
O	0.3538921	-4.0102359	1.0347936	O	0.4197581	-4.0846882	1.1407468	C	2.4786081	-1.2611261	-1.8706324
C	2.1676281	1.1336262	0.1073566	C	2.2585711	0.9947865	-0.0774041	H	-0.5501035	-1.5049497	1.6039271
H	1.7241249	1.4642657	-0.8419236	H	1.8373368	1.3075567	-1.0424048	C	1.1508150	-5.5526093	0.0859621
H	1.8284164	1.7905985	0.9120967	H	1.9471588	1.6994510	0.6963384	H	0.5037087	-5.9312889	0.8810630
H	3.2602560	1.1660867	0.0181160	H	3.3511239	0.9678219	-0.1579395	H	0.8348235	-5.9585164	-0.8829989
C	1.9503917	-3.5397445	-1.1798744	C	2.0915446	-3.7606703	-1.0542798	H	2.1913799	-5.8440163	0.2746947
H	1.5767951	-4.4931938	-0.7973416	H	1.6604481	-4.6806120	-0.6513695	H	3.0370294	-1.9792894	-2.4745949
H	1.4691655	-3.3125583	-2.1411642	H	1.7127060	-3.5818109	-2.0689802	H	1.8085525	-0.6743689	-2.5097609
H	3.0354321	-3.5881024	-1.3311340	H	3.1850962	-3.8371986	-1.0916775	H	3.1704133	-0.5872966	-1.3520528

MB + 1a

N-E

C	-1.0234933	-0.8627355	-2.5744600
C	-0.1198573	-0.5878518	-1.5482490
C	-0.1682391	0.6326271	-0.8555392
C	-1.1276186	1.5777436	-1.2424071
C	-2.0326248	1.3016390	-2.2721968
C	-2.0061069	0.0719127	-2.9471485
H	-0.9707982	-1.8227595	-3.0932940
H	0.6304399	-1.3322617	-1.2731050
H	-1.1770244	2.5383014	-0.7233008

H	-2.7737806	2.0540332	-2.5513315
C	0.7156534	0.8877755	0.3555751
C	2.1764321	0.4921289	0.1504503
C	2.7824594	0.8269513	-1.0751852
C	2.9825208	-0.0922124	1.1358026
C	4.1363982	0.5819847	-1.3046768
H	2.1826598	1.2898363	-1.8612324
C	4.3407438	-0.3401357	0.9018063
H	2.5619348	-0.3842014	2.0965993
C	4.9446835	-0.0130903	-0.3202015
H	4.5747732	0.8592188	-2.2666541
H	4.9392765	-0.8017309	1.6910389
H	0.7131515	1.9733714	0.5501798
C	-3.0143419	-0.2535817	-4.0204063
H	-2.5618283	-0.8398923	-4.8328615
H	-3.8384920	-0.8554565	-3.6042678
H	-3.4539969	0.6566426	-4.4506451
C	6.3995596	-0.3129100	-0.5851138
H	6.9618568	-0.4359226	0.3507678
H	6.5072318	-1.2459740	-1.1617021
H	6.8729758	0.4872854	-1.1722628
C	0.0332778	0.2833226	1.6603659
C	-1.1765733	1.1430395	1.9543010
C	-0.2409217	-1.1933599	1.4998983
N	-2.3974807	0.6590972	1.5098771
O	-1.0592058	2.2499739	2.4776821
N	-1.5171015	-1.5286898	1.0558295
O	0.6271623	-2.0436821	1.6795918
C	-2.5770997	-0.6189857	0.9562524
O	-3.6496111	-0.9468676	0.4638613
C	-1.7977027	-2.8953970	0.5894273
H	-0.8973482	-3.4929702	0.7496335
H	-2.6375069	-3.3188571	1.1514689
H	-2.0480015	-2.8656896	-0.4783813
C	-3.5821414	1.5320312	1.5118035
H	-4.4049221	1.0417990	2.0433844
H	-3.3093558	2.4632700	2.0135691
H	-3.8847767	1.7347096	0.4767507
H	0.7235484	0.4139637	2.5019252

B + 2a											
$N^{\ominus}+E$				TS_c				$N-E^{\ominus}$			
C	-0.0874651	-0.9346879	0.7387402	C	-0.0430671	-0.8179558	0.4247099	C	-0.3981065	0.1526492	0.1651779
C	-1.3133547	-0.3786518	0.4196017	C	-1.3638378	-0.3013256	0.2181546	C	1.0694425	0.0554941	-0.1660004
C	-2.2482676	-1.3094105	-0.2595392	C	-2.3115169	-1.2699285	-0.3068666	C	1.6414433	1.1451226	-0.8799129
C	-1.7161264	1.0309650	0.5137714	C	-1.7653775	1.0840609	0.2898928	C	1.8083465	-1.1348739	0.0497325
C	-4.0084017	0.2093292	0.4080544	C	-4.0533803	0.2495706	0.3997065	C	3.7995748	0.2002753	-0.3090138

C	1.1315639	-0.5071545	1.4008790	C	1.0485871	-0.3287284	1.2984404	C	-0.7101730	0.2422899	1.6509658
C	2.0875218	-1.5317068	1.6329235	C	1.8007281	-1.3231937	1.9661060	C	-1.2926731	1.4199169	2.1458042
C	1.4683354	0.8111939	1.7880663	C	1.4507851	1.0138905	1.4489967	C	-0.4410351	-0.8036638	2.5494725
C	3.3161959	-1.2548817	2.2249088	C	2.8951342	-0.9909561	2.7653386	C	-1.5861043	1.5623209	3.5072042
H	1.8572082	-2.5515010	1.3207176	H	1.5225858	-2.3714710	1.8430072	H	-1.5163930	2.2375143	1.4559846
C	2.6997775	1.0823194	2.3808945	C	2.5513591	1.3434746	2.2429307	C	-0.7342896	-0.6648597	3.9084903
H	0.7667574	1.6146225	1.5849266	H	0.8944092	1.7873049	0.9277724	H	0.0040194	-1.7239077	2.1721021
C	3.6291343	0.0576220	2.6007566	C	3.2788811	0.3479237	2.9046637	C	-1.3064653	0.5182862	4.3949214
H	4.0358897	-2.0592349	2.3842616	H	3.4548658	-1.7793404	3.2718866	H	-2.0347493	2.4886215	3.8719614
H	2.9454610	2.1083082	2.6591230	H	2.8497557	2.3893879	2.3355013	H	-0.5177862	-1.4869937	4.5941155
H	4.5953200	0.2814063	3.0566739	H	4.1409403	0.6118412	3.5201880	H	-1.5352504	0.6230905	5.4572977
O	-0.9888651	2.0018322	0.6841640	O	-1.0517691	2.0834569	0.3859540	O	1.3824319	-2.2378911	0.4363140
O	-1.9497930	-2.4036180	-0.7219104	O	-2.0355681	-2.3981279	-0.7277594	O	1.0524187	2.1387999	-1.3414328
O	-3.0547091	1.2991322	0.3353839	O	-3.1314495	1.3413737	0.1860863	O	3.1775502	-1.1030788	-0.2638378
O	-3.5451001	-0.8922572	-0.4156321	O	-3.6391441	-0.8912503	-0.3941789	O	3.0177846	1.0899139	-1.1399815
C	-5.2813755	0.7152727	-0.2365380	C	-5.3874126	0.6977518	-0.1630597	C	5.1312732	0.0176092	-1.0125615
H	-6.0365992	-0.0804398	-0.2341681	H	-6.1249025	-0.1073363	-0.0531581	H	5.6428957	0.9849617	-1.0971703
H	-5.6647699	1.5727072	0.3302862	H	-5.7406410	1.5810583	0.3837725	H	5.7642474	-0.6699726	-0.4370498
H	-5.0774081	1.0223348	-1.2698284	H	-5.2768966	0.9477844	-1.2257816	H	4.9667312	-0.3948005	-2.0163160
C	-4.1901843	-0.2454481	1.8515759	C	-4.1178161	-0.1232578	1.8789679	C	3.9455462	0.7752058	1.1011570
H	-4.5572997	0.5949788	2.4538194	H	-4.4533335	0.7464466	2.4581864	H	4.5626878	0.1003684	1.7085094
H	-4.9232662	-1.0610451	1.8871499	H	-4.8330555	-0.9439609	2.0180945	H	4.4352711	1.7562507	1.0475288
H	-3.2426170	-0.6004895	2.2778075	H	-3.1345955	-0.4401490	2.2493467	H	2.9647278	0.8901052	1.5795724
H	-0.0656863	-2.0020445	0.5039731	H	-0.0722793	-1.9104293	0.4377929	H	-0.7366280	1.0984300	-0.2834628
C	0.9818501	-0.9803188	-1.9165361	C	0.8518299	-0.9525616	-1.4924321	C	-1.2621872	-0.9936598	-0.5507785
C	0.3527087	0.2839621	-1.9974250	C	0.6093005	0.3770723	-2.0054278	C	-2.7044930	-0.8289095	-0.1458802
C	2.3372086	-1.1304559	-1.5274140	C	2.2016181	-1.3814502	-1.1988123	C	-1.0341019	-0.8434380	-2.0343281
N	1.1575897	1.3928613	-1.6261656	N	1.6580097	1.2950383	-1.8088259	N	-3.4127937	0.1121344	-0.8931733
O	-0.8417712	0.5057706	-2.3142487	O	-0.4548914	0.7519054	-2.5199930	O	-3.2245735	-1.3968080	0.8084019
N	3.0109012	0.0754334	-1.2038649	N	3.1457684	-0.3473505	-1.0943411	N	-1.8771946	0.0721485	-2.6638223
O	2.9749329	-2.2053538	-1.4245754	O	2.5498046	-2.5537900	-0.9770054	O	-0.1318472	-1.3963657	-2.6515031
C	2.4702005	1.3455675	-1.2112644	C	2.9334675	0.9943444	-1.3666799	C	-3.0632169	0.5846258	-2.1540764
O	3.1151208	2.3545606	-0.8861951	O	3.8186902	1.8464645	-1.2452967	O	-3.7714319	1.3650852	-2.7851023
H	0.3991077	-1.8650933	-2.1574286	H	0.1675491	-1.7246712	-1.8399742	H	-0.8860383	-1.9660553	-0.2174695
H	0.6937786	2.2980097	-1.5751532	H	1.4847932	2.2666825	-2.0634936	H	-4.3542201	0.3521867	-0.5790848
H	3.9668680	-0.0082429	-0.8627351	H	4.0837052	-0.6001426	-0.7856400	H	-1.6740621	0.3093858	-3.6356958

B + 2a						
TS _{PT}				Θ _{N-E}		
C	-0.1825890	-0.6836074	-0.5088159	C	0.1459972	0.0415535
C	-0.1570382	-0.4152099	-1.9937104	C	0.0621507	0.3014778
C	1.0487251	-0.2130503	-2.6791547	C	0.6006742	-0.6569164
C	1.0714545	-0.0813728	-4.0724868	C	0.5327667	-0.4863493
C	-0.1185802	-0.1525676	-4.8051396	C	-0.0704277	0.6571723
C	-1.3288255	-0.3607125	-4.1301689	C	-0.6032393	1.6228308
C	-1.3451000	-0.4893856	-2.7389460	C	-0.5362740	1.4488650
H	1.9839132	-0.1529746	-2.1205814	H	1.0749942	-1.5511750

H	2.0221653	0.0800755	-4.5846428	H	0.9555445	-1.2449905	-4.8668028
H	-0.1042387	-0.0476196	-5.8915658	H	-0.1234708	0.7969816	-5.8208340
H	-2.2647408	-0.4177748	-4.6898172	H	-1.0732883	2.5198263	-4.2839531
H	-2.2936513	-0.6439725	-2.2208002	H	-0.9625215	2.1932241	-1.8179347
C	-1.3877304	-0.2057146	0.3404395	C	-1.1653032	-0.2914918	0.2134462
C	-2.0769291	1.0579600	0.0859710	C	-2.1628779	0.6908912	0.4439934
N	-3.1160080	1.3585329	1.0044212	N	-3.3335307	0.2400190	1.1166167
C	-3.7043521	0.4948944	1.9032721	C	-3.5748901	-1.0299623	1.5863882
N	-3.1653164	-0.7773028	1.8950048	N	-2.5437060	-1.9115748	1.3506760
C	-2.1257167	-1.2405506	1.0660393	C	-1.3137066	-1.6181821	0.7060439
O	-1.8324915	1.8746914	-0.8060833	O	-2.1169145	1.9060995	0.1303683
O	-4.6462473	0.8194974	2.6371732	O	-4.6239003	-1.3529940	2.1707135
O	-1.8793050	-2.4562766	1.0477249	O	-0.4681030	-2.5475454	0.6275479
H	-3.6304560	-1.4709406	2.4798971	H	-2.6664062	-2.8631061	1.6934333
H	-3.5574121	2.2721497	0.9019176	H	-4.0598443	0.9354093	1.2815330
H	-0.1827195	-1.7789325	-0.3832535	H	0.7501569	-0.8667676	-0.3362725
H	-0.2069060	0.0918922	1.1458324	H	0.3491588	2.1241054	0.1771592
C	0.9841586	-0.1969019	0.3898168	C	0.9277424	1.2024448	0.3113286
C	1.7252169	-1.2210242	1.1247399	C	0.9924792	0.9319139	1.7963799
O	2.7926945	-0.7863729	1.8988606	O	2.1231093	0.3432684	2.2873115
C	3.5436659	0.3530692	1.4073978	C	3.1924017	-0.1495635	1.4299985
O	2.6489627	1.4366434	1.0584976	O	3.3131508	0.6416191	0.2031682
C	1.5487252	1.1432733	0.2532346	C	2.2880262	1.3791411	-0.3120923
O	1.0899681	2.0606207	-0.4118662	O	2.5175185	2.1053310	-1.2611822
O	1.4273548	-2.4094120	1.2029299	O	0.1154714	1.2341471	2.5812619
C	4.3880071	0.8450031	2.5644165	C	4.4799143	0.0988077	2.1927876
C	4.3589972	-0.0593184	0.1856354	C	2.9556514	-1.6137611	1.0989591
H	5.0765617	0.0524671	2.8832373	H	4.4497829	-0.4388554	3.1485000
H	4.9721249	1.7187575	2.2493990	H	5.3298780	-0.2664256	1.6029888
H	3.7398675	1.1243402	3.4046463	H	4.6005056	1.1729380	2.3802828
H	4.9238918	0.8028048	-0.1903557	H	3.7011299	-1.9445567	0.3651272
H	5.0580166	-0.8594040	0.4599097	H	3.0704200	-2.2074328	2.0148467
H	3.7030183	-0.4280857	-0.6149908	H	1.9463688	-1.7897197	0.7066889

B + 2a

N _O [⊖] +E				TS _O			N _O -E [⊖]				
C	-1.4687242	-0.5089497	-1.0731102	C	-0.4298246	-1.1083310	-1.0884237	C	0.8080937	-0.6493810	-0.3846824
C	-1.2250600	-0.0847726	0.2143016	C	0.7736559	-0.6597864	-0.4358409	C	-0.5314776	-0.1285300	-0.7932660
C	-0.5733534	1.1683377	0.6344490	C	0.8357454	-0.3804110	0.9726461	C	-0.7012826	1.2494789	-1.1052061
C	-1.6225572	-1.0600862	1.2712996	C	1.8930568	-0.3236643	-1.2797209	C	-1.6213723	-1.0410364	-0.8421029
C	-1.4853250	0.7657392	2.8671218	C	3.2469928	-0.5078073	0.7241649	C	-2.7328539	0.5885385	-2.2491437
C	-1.2192202	-0.0312363	-2.4201862	C	-1.2327626	-2.2463123	-0.5364125	C	1.8649202	-0.5060281	-1.4608223
C	-0.3341818	1.0047614	-2.8063964	C	-2.0842604	-2.1442567	0.5756626	C	2.7049669	0.6119848	-1.5584170
C	-1.9014425	-0.7374037	-3.4472910	C	-1.1025703	-3.4911361	-1.1787770	C	1.9519015	-1.5159049	-2.4325109
C	-0.1577169	1.3193271	-4.1531138	C	-2.7691777	-3.2678228	1.0468154	C	3.6177691	0.7159354	-2.6144381
H	0.2110849	1.5448725	-2.0383467	H	-2.1969365	-1.1812897	1.0664363	H	2.6273878	1.4012314	-0.8132269
C	-1.7361322	-0.4053742	-4.7892274	C	-1.7779987	-4.6182605	-0.6989826	C	2.8587448	-1.4082991	-3.4908652

H	-2.5717397	-1.5548797	-3.1731718	H	-0.4589127	-3.5791212	-2.0571929	H	1.2991641	-2.3894545	-2.3613944
C	-0.8583921	0.6257755	-5.1490562	C	-2.6149738	-4.5099148	0.4173354	C	3.6972467	-0.2901037	-3.5845789
H	0.5371965	2.1138451	-4.4306423	H	-3.4298590	-3.1725098	1.9108291	H	4.2686518	1.5902197	-2.6804408
H	-2.2799629	-0.9573760	-5.5573470	H	-1.6588575	-5.5776059	-1.2059823	H	2.9163864	-2.2017104	-4.2384948
H	-0.7166212	0.8828455	-6.2002376	H	-3.1509561	-5.3850929	0.7892740	H	4.4096815	-0.2056312	-4.4073422
H	-1.9986962	-1.4655588	-1.0768313	H	-0.2460228	-1.2392569	-2.1585278	H	0.6989359	-1.7151408	-0.1354929
O	-1.9913077	-2.2081322	1.0656329	O	1.8846011	-0.2110215	-2.5115057	O	-1.6433293	-2.2133350	-0.4256292
O	-0.0061557	1.9765263	-0.0877987	O	-0.1142138	-0.2822535	1.7518817	O	0.1083868	2.1678738	-0.9282089
O	-1.5251304	-0.6542109	2.5722567	O	3.0976645	-0.0562991	-0.6477181	O	-2.8225838	-0.5668421	-1.3766146
O	-0.5599325	1.4395924	1.9771639	O	2.0945836	-0.1031213	1.5009974	O	-1.9573083	1.6283805	-1.6116379
C	-0.8967484	0.8924618	4.2548674	C	4.4313113	0.2489192	1.2913508	C	-4.1434646	1.1267612	-2.3898128
H	-0.8373320	1.9522809	4.5325150	H	4.5816979	-0.0331378	2.3410903	H	-4.1374753	2.0195099	-3.0281180
H	-1.5378137	0.3697347	4.9756844	H	5.3365170	0.0008948	0.7228259	H	-4.7876215	0.3659008	-2.8487505
H	0.1086767	0.4514740	4.2531664	H	4.2456766	1.3285133	1.2276034	H	-4.5406339	1.3902940	-1.4011820
C	-2.8773335	1.3617478	2.7074888	C	3.4208997	-2.0241426	0.7697124	C	-2.1054771	0.1951936	-3.5871347
H	-3.5719006	0.8605162	3.3931115	H	4.3087127	-2.3077556	0.1901644	H	-2.7165664	-0.5818354	-4.0641985
H	-2.8466643	2.4328306	2.9431198	H	3.5558266	-2.3432915	1.8111278	H	-2.0667719	1.0738507	-4.2439230
H	-3.2400816	1.2342555	1.6778870	H	2.5435162	-2.5338342	0.3518109	H	-1.0868025	-0.1883694	-3.4449776
O	0.8334372	-2.3956837	-1.0397729	O	-1.6654121	0.1401602	-1.1988384	O	1.3683524	0.0271802	0.8281356
C	1.3901180	-1.5578331	-0.2886828	C	-1.3590456	1.3354567	-0.7576469	C	0.7339930	-0.0984354	1.9894217
N	2.0537225	-0.4632110	-0.9086354	N	-2.2448129	1.8377648	0.1952372	N	1.2740835	0.7480025	2.9406524
C	1.4032606	-1.5519697	1.1244000	C	-0.2819893	2.1068895	-1.1448058	C	-0.3078574	-0.9346699	2.3115801
C	2.6819995	0.5821245	-0.2684755	C	-2.1086565	3.0543696	0.8344781	C	0.8409858	0.8218807	4.2553467
C	2.0371854	-0.5332100	1.8767436	C	-0.0464622	3.3855001	-0.5472562	C	-0.8353295	-0.9311394	3.6454459
H	0.8956467	-2.3533522	1.6539004	H	0.4000944	1.7489919	-1.9094702	H	-0.7539349	-1.6035859	1.5801815
N	2.6471832	0.4970312	1.1075311	N	-0.9968604	3.7693350	0.4316927	N	-0.2072970	-0.0295751	4.5393006
O	3.2365626	1.5113883	-0.8771798	O	-2.9065435	3.4594953	1.6897506	O	1.3518209	1.5832148	5.0821651
O	2.1042222	-0.4469573	3.1272829	O	0.8888118	4.1654863	-0.8117574	O	-1.7696409	-1.6380884	4.0642349
H	3.0905772	1.2556589	1.6224187	H	-3.0176586	1.2422995	0.4872150	H	-0.5601813	-0.0074169	5.4960548
H	2.0177097	-0.4214578	-1.9254987	H	-0.8624983	4.6790898	0.8725331	H	2.0450247	1.3575363	2.6708339

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N [⊖] +E				TS _C			N-E [⊖]				
C	-0.3444283	-0.4858920	1.1595485	C	-0.2607875	-0.5893771	0.8986882	C	-0.8068726	-0.5068601	0.8809971
C	-1.5665961	-0.1529515	0.5870019	C	-1.5618064	-0.2222507	0.4466705	C	-0.3555648	0.6496739	0.0290807
C	-2.4683657	-1.3037710	0.3650537	C	-2.4975457	-1.3344455	0.3428690	C	-1.2681140	1.2051599	-0.9064027
C	-1.9861095	1.1521838	0.0771652	C	-1.9618042	1.0615964	-0.0851181	C	0.9823231	1.1166063	0.1245648
C	-4.2679525	0.3041854	0.2090928	C	-4.2561337	0.3228802	0.2765015	C	0.2503057	3.0885554	-1.0814741
C	0.8405649	0.2311824	1.6015144	C	0.8342739	0.2145611	1.4739325	C	-0.4980878	-0.3065249	2.3632358
C	1.6864654	-0.4789587	2.4941434	C	1.5911669	-0.4107911	2.4937869	C	-1.0409214	0.8408992	2.9713068
C	1.2600820	1.5128233	1.1751836	C	1.2428799	1.4937233	1.0420790	C	0.2454426	-1.1887334	3.1570234
C	2.8664984	0.0815430	2.9741419	C	2.6882978	0.2230192	3.0762255	C	-0.8424203	1.1039169	4.3280718
H	1.4040135	-1.4871966	2.8015325	H	1.3127039	-1.4140518	2.8209426	H	-1.6251581	1.5358299	2.3636391
C	2.4514050	2.0626302	1.6463182	C	2.3498991	2.1203081	1.6176501	C	0.4480919	-0.9277147	4.5196170
H	0.6464870	2.0547763	0.4624959	H	0.6878994	1.9780157	0.2441709	H	0.7010193	-2.0739259	2.7150496
C	3.2548625	1.3594577	2.5524163	C	3.0759111	1.4944341	2.6375131	C	-0.0922118	0.2169228	5.1125628
H	3.4948642	-0.4838665	3.6640192	H	3.2502157	-0.2818800	3.8639222	H	-1.2769097	2.0002010	4.7757404

H	2.7640934	3.0454985	1.2905108	H	2.6554644	3.1034183	1.2553640	H	1.0383762	-1.6258364	5.1170909
H	4.1866733	1.7970269	2.9151888	H	3.9427853	1.9884428	3.0801719	H	0.0678466	0.4184516	6.1734390
O	-1.2891680	2.1448373	-0.1053331	O	-1.2478711	2.0185968	-0.3885555	O	1.8985861	0.6068869	0.7843074
O	-2.1506700	-2.4846878	0.4603718	O	-2.2129917	-2.5303549	0.4489259	O	-2.4072613	0.7900036	-1.1796589
O	-3.3140072	1.2772726	-0.2798767	O	-3.3194032	1.2346274	-0.3391069	O	1.3313009	2.2289043	-0.6545865
O	-3.7569501	-1.0334946	-0.0245176	O	-3.8167017	-1.0410178	0.0538164	O	-0.8272484	2.3075217	-1.6498372
C	-5.5031628	0.4452499	-0.6552453	C	-5.5627258	0.4774350	-0.4756053	C	0.8001650	3.9402789	-2.2096158
H	-6.2560503	-0.2899854	-0.3450607	H	-6.3092269	-0.2152705	-0.0670145	H	0.0157563	4.6072852	-2.5896759
H	-5.9201470	1.4533214	-0.5390582	H	-5.9324001	1.5046745	-0.3655872	H	1.6371375	4.5481312	-1.8427264
H	-5.2410061	0.2778335	-1.7073633	H	-5.4066157	0.2588143	-1.5395199	H	1.1514535	3.2911776	-3.0217539
C	-4.5325708	0.5177250	1.6955494	C	-4.3825167	0.6058090	1.7713864	C	-0.2627328	3.9136888	0.0993438
H	-4.9352963	1.5262872	1.8521219	H	-4.7360641	1.6344038	1.9176978	H	0.5546814	4.5253024	0.5027927
H	-5.2647275	-0.2205629	2.0459836	H	-5.1072114	-0.0888840	2.2148253	H	-1.0733869	4.5735617	-0.2359640
H	-3.6100017	0.4088119	2.2809776	H	-3.4167816	0.4856679	2.2787773	H	-0.6411000	3.2580047	0.8940311
H	-0.3286306	-1.5291991	1.4832472	H	-0.2844272	-1.5837614	1.3501596	H	-1.9067574	-0.5206146	0.8058582
C	0.8005766	-1.7075720	-0.9673319	C	0.7022993	-1.5591321	-0.8252696	C	-0.4071665	-1.9479706	0.3122295
C	0.3336409	-0.6313500	-1.7554328	C	0.3870831	-0.5778425	-1.8226369	C	-1.2954569	-2.1764477	-0.8889415
C	2.1216394	-1.7896521	-0.4643827	C	2.0486750	-1.7537473	-0.3647911	C	1.0604846	-2.0984246	-0.0014129
N	1.2519601	0.4328603	-1.9714752	N	1.3619508	0.4190624	-2.0393252	N	-0.7928827	-1.6996847	-2.0898074
O	-0.8270025	-0.5270678	-2.2210657	O	-0.7037524	-0.5174907	-2.4185770	O	-2.4164945	-2.6763248	-0.7886898
N	2.9610691	-0.6773340	-0.7628467	N	2.9567694	-0.7215479	-0.6907465	N	1.4415251	-1.5738556	-1.2339503
O	2.5723240	-2.7369159	0.2227607	O	2.4132378	-2.7213185	0.3313411	O	1.8668222	-2.6316960	0.7599604
C	2.5647732	0.4253167	-1.5140300	C	2.6483256	0.3702449	-1.5054041	C	0.5289518	-1.2472401	-2.2439172
O	3.3611299	1.3462241	-1.7568756	O	3.4970421	1.2370207	-1.7448596	O	0.8926260	-0.7007189	-3.2812006
C	4.3360642	-0.6546833	-0.2601854	C	4.3061633	-0.7351190	-0.1166260	C	2.8593760	-1.3254860	-1.5257372
H	5.0518870	-0.6680897	-1.0931074	H	5.0612098	-0.7879698	-0.9110410	H	3.1932417	-1.9510822	-2.3629552
H	4.4966886	0.2509542	0.3369921	H	4.4607873	0.1774390	0.4720918	H	2.9917029	-0.2675403	-1.7782575
H	4.4679176	-1.5414069	0.3652321	H	4.3769716	-1.6131314	0.5301410	H	3.4268797	-1.5668022	-0.6242563
C	0.7684233	1.5900824	-2.7287927	C	0.9824276	1.5521673	-2.8892560	C	-1.6713152	-1.5663710	-3.2598707
H	1.5764122	2.3233975	-2.7868489	H	1.7891745	2.2884077	-2.8616500	H	-1.8466162	-0.5029272	-3.4614710
H	0.4683094	1.2818035	-3.7389316	H	0.8182743	1.2163316	-3.9215894	H	-1.2078547	-2.0426288	-4.1309726
H	-0.0989335	2.0209430	-2.2137433	H	0.0545969	1.9851193	-2.4958712	H	-2.6177960	-2.0562456	-3.0186301
H	0.1238474	-2.5384398	-0.7873744	H	0.0427622	-2.4233179	-0.7794050	H	-0.6768911	-2.7006075	1.0616274

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C	0.2215278	-0.7423646	-0.5941397	C	0.5193293	0.1942278	-0.4821195
C	0.5203802	-0.5239887	-2.0569158	C	0.6420336	0.4782507	-1.9741664
C	1.8131369	-0.2322531	-2.5112870	C	0.9195694	-0.6041662	-2.8263352
C	2.0927408	-0.1445683	-3.8806840	C	0.9982213	-0.4304864	-4.2124971
C	1.0776189	-0.3519996	-4.8205822	C	0.8095781	0.8396708	-4.7692397
C	-0.2179107	-0.6517997	-4.3767392	C	0.5427941	1.9267772	-3.9271154
C	-0.4905110	-0.7355813	-3.0095919	C	0.4618516	1.7491078	-2.5424543
H	2.6143747	-0.0656075	-1.7901736	H	1.0670000	-1.5977295	-2.3954404
H	3.1069763	0.0888918	-4.2111099	H	1.2137003	-1.2861703	-4.8556968
H	1.2920441	-0.2819450	-5.8886342	H	0.8737539	0.9825245	-5.8496980
H	-1.0196436	-0.8156511	-5.0998644	H	0.3993151	2.9226465	-4.3519398

H	-1.5043760	-0.9597503	-2.6713272	H	0.2404864	2.5963839	-1.8964194
C	-1.1334554	-0.2700735	-0.0009285	C	-0.9025112	0.0150005	-0.0181525
C	-1.7872201	0.9522835	-0.4551618	C	-1.7885494	1.1175582	0.0369479
N	-2.9596348	1.3087468	0.2764111	N	-3.1123904	0.8412542	0.5117010
C	-3.6430792	0.4475984	1.1211126	C	-3.5392202	-0.4046706	0.9335607
N	-3.1422734	-0.8445493	1.2496305	N	-2.6144118	-1.4351591	0.8870228
C	-1.9665257	-1.3033930	0.6106261	C	-1.2667805	-1.2785751	0.4393900
O	-1.3986919	1.6819216	-1.3710256	O	-1.5004527	2.2968825	-0.2846790
C	-3.5741283	2.6216625	0.0437268	C	-4.0940780	1.9264992	0.5865469
O	-4.6785612	0.7954653	1.7059896	O	-4.7010397	-0.5932480	1.3409211
C	-3.9449520	-1.7769173	2.0521023	C	-3.0785070	-2.7468882	1.3487100
O	-1.6768177	-2.5102141	0.6467297	O	-0.5014800	-2.2789141	0.4770813
H	-2.8697989	3.2186942	-0.5413996	H	-3.6084825	2.8327627	0.2144944
H	-4.5164420	2.5182074	-0.5115037	H	-4.9718973	1.6893863	-0.0288019
H	-3.7782104	3.1061036	1.0054844	H	-4.4213711	2.0763550	1.6240906
H	-3.3987558	-2.7217329	2.1088042	H	-2.2462446	-3.4468924	1.2374056
H	-4.0957293	-1.3645450	3.0568886	H	-3.3859865	-2.6954066	2.4017173
H	-4.9239405	-1.9422578	1.5834117	H	-3.9348974	-3.0799836	0.7479412
H	-0.1322268	0.0743837	1.0042897	H	0.9057755	2.2275590	0.2081132
C	1.1849026	-0.1976014	0.4897115	C	1.3267889	1.2351214	0.4077501
C	1.8211020	-1.1799063	1.3640696	C	1.1223933	0.9664198	1.8806197
O	2.7155571	-0.6916047	2.3087408	O	2.0808454	0.2482333	2.5379141
C	3.4971516	0.4710167	1.9352595	C	3.1946702	-0.3891861	1.8495993
O	2.6361901	1.5134780	1.4170247	O	3.6104381	0.3750779	0.6716232
C	1.7012278	1.1671364	0.4415568	C	2.7784160	1.2256294	0.0045019
O	1.3121799	2.0642112	-0.2929008	O	3.2444612	1.9012304	-0.8945172
O	1.5622925	-2.3796924	1.4121274	O	0.1773507	1.3823079	2.5213828
C	4.1065406	1.0098543	3.2129479	C	4.3683473	-0.3146822	2.8076761
C	4.5299680	0.0796014	0.8825798	C	2.8171730	-1.8080528	1.4586524
H	4.7586299	0.2497826	3.6612602	H	4.1167887	-0.8396772	3.7374594
H	4.7026986	1.9034346	2.9892650	H	5.2431859	-0.7943233	2.3512408
H	3.3110337	1.2714967	3.9220823	H	4.6018162	0.7337978	3.0305746
H	5.1162711	0.9609437	0.5940488	H	3.6154498	-2.2383270	0.8410514
H	5.2024169	-0.6855346	1.2905287	H	2.7092095	-2.4101152	2.3700118
H	4.0400334	-0.3275537	-0.0125950	H	1.8647834	-1.8454489	0.9151754
H	0.2198159	-1.8322687	-0.4311169	H	0.9901534	-0.7832470	-0.3257171

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$N_O^{\ominus}+E$				TS_O			$N_O-E^{\ominus}$				
C	-1.0827217	-0.7609302	-1.6432197	C	-0.4144989	-1.1109470	-1.4567053	C	0.1660580	-0.7705170	-1.0752558
C	-1.3903069	-0.2908581	-0.3907876	C	-1.2631091	-0.4655938	-0.5003715	C	-0.9989488	0.0276640	-0.5872311
C	-0.9075903	0.9822629	0.1866447	C	-0.9778955	0.8610387	-0.0076980	C	-0.9244369	1.4467953	-0.5376507
C	-2.0829363	-1.2511609	0.5087193	C	-2.2300621	-1.2852514	0.1872428	C	-2.1373362	-0.6743975	-0.1040383
C	-2.5681826	0.6537679	1.9394909	C	-3.2021825	0.7997854	0.9605971	C	-3.3416679	1.4136971	-0.3583850
C	-0.4567217	-0.1553801	-2.8046526	C	0.0890054	-0.4206263	-2.6834473	C	0.4849624	-0.5446885	-2.5387043
C	-0.4883416	1.2219414	-3.1147834	C	-0.4993084	0.7652934	-3.1528196	C	-0.1926360	-1.3230582	-3.4906938
C	0.1927393	-1.0328359	-3.7057758	C	1.1067863	-1.0142854	-3.4533201	C	1.3764355	0.4462720	-2.9740601

C	0.1440141	1.7030271	-4.2599403	C	-0.0596016	1.3614912	-4.3385776	C	0.0092195	-1.1098194	-4.8575406
H	-1.0167325	1.9124263	-2.4623895	H	-1.3127701	1.2226058	-2.5906554	H	-0.8875888	-2.0975511	-3.1569533
C	0.8462803	-0.5453972	-4.8353927	C	1.5529740	-0.4165892	-4.6332611	C	1.5831478	0.6550735	-4.3424391
H	0.2166906	-2.0989960	-3.4757462	H	1.5681218	-1.9371198	-3.1020570	H	1.8922322	1.0558702	-2.2350210
C	0.8275569	0.8271913	-5.1150147	C	0.9743651	0.7787955	-5.0796874	C	0.9002908	-0.1186214	-5.2885741
H	0.1054463	2.7692518	-4.4894120	H	-0.5285071	2.2849351	-4.6838140	H	-0.5233004	-1.7234324	-5.5867528
H	1.3665093	-1.2343929	-5.5026787	H	2.3527806	-0.8861576	-5.2091529	H	2.2808406	1.4282628	-4.6708502
H	-1.3537128	-1.8106055	-1.7835441	H	-0.7472989	-2.1316634	-1.6606086	H	-0.0594302	-1.8359817	-0.9207210
O	-2.3115982	-2.4254598	0.2493344	O	-2.3596860	-2.5111953	0.0985149	O	-2.2435883	-1.8977578	0.0908061
O	-0.0703471	1.7226798	-0.3041196	O	0.0183397	1.5415942	-0.2541656	O	0.0717460	2.1588795	-0.7257809
O	-2.4825905	-0.7822012	1.7286502	O	-3.0817692	-0.6420040	1.0734818	O	-3.2570514	0.0927015	0.2341861
O	-1.3781560	1.3091933	1.4318662	O	-1.8876008	1.4017062	0.8943899	O	-2.0977040	2.1239417	-0.1612235
C	-2.5497842	0.8607112	3.4377782	C	-3.8223099	1.2751689	2.2593145	C	-4.3967416	2.1665075	0.4289312
H	-2.6046895	1.9339616	3.6590911	H	-3.9218514	2.3678641	2.2432949	H	-4.4937110	3.1871339	0.0372767
H	-3.4138598	0.3576196	3.8897057	H	-4.8171335	0.8284048	2.3810637	H	-5.3641488	1.6566051	0.3359584
H	-1.6166835	0.4437501	3.8384234	H	-3.1845956	0.9804815	3.1021913	H	-4.1095947	2.2097859	1.4873619
C	-3.8036871	1.2038486	1.2386590	C	-4.0234073	1.1698579	-0.2725036	C	-3.6692194	1.3077290	-1.8483772
H	-4.7012593	0.7204096	1.6441183	H	-5.0263366	0.7319236	-0.1899408	H	-4.6245337	0.7825928	-1.9767461
H	-3.8685899	2.2859111	1.4083290	H	-4.1128094	2.2618623	-0.3362062	H	-3.7545361	2.3153533	-2.2754399
H	-3.7572585	1.0160564	0.1569319	H	-3.5466918	0.7968871	-1.1880445	H	-2.8845258	0.7586369	-2.3845017
H	2.9292190	1.7749684	3.2398688	H	3.3956483	0.9125258	4.2258239	H	3.1141682	-0.9018867	5.3508410
O	1.2020138	-2.3897142	-0.7808905	O	1.1215906	-1.6522227	-0.6902553	O	1.4279293	-0.4639224	-0.3370363
C	1.3718827	-1.5590910	0.1483153	C	1.3862623	-1.1132702	0.4725057	C	1.4368580	-0.5586687	0.9926142
N	2.1705569	-0.3994827	-0.0967065	N	2.3944206	-0.1413784	0.4988420	N	2.4202851	0.2341566	1.5582674
C	0.8051661	-1.6501067	1.4357168	C	0.7223592	-1.4364401	1.6367041	C	0.6179623	-1.3415565	1.7656151
C	2.3655335	0.6105400	0.8326499	C	2.6828854	0.5911943	1.6441730	C	2.6633396	0.2289704	2.9352855
C	0.9649766	-0.6691683	2.4392518	C	0.9909169	-0.7720487	2.8698926	C	0.7742632	-1.3797565	3.1843002
H	0.1875883	-2.5154793	1.6605556	H	-0.0487753	-2.2008703	1.6125059	H	-0.1714665	-1.9419259	1.3214365
N	1.7481806	0.4666617	2.0673189	N	1.9903692	0.2390517	2.8009545	N	1.8330397	-0.5774803	3.7033579
O	3.0655774	1.6047788	0.5734723	O	3.5179990	1.5083600	1.6539554	O	3.5597154	0.9117851	3.4456642
O	0.4699561	-0.7207087	3.5933697	O	0.4193571	-1.0147959	3.9526432	O	0.0729871	-2.0609943	3.9573419
C	2.7309805	-0.1728952	-1.4293453	C	3.0018921	0.2777528	-0.7707884	C	3.1904057	1.1468620	0.6957811
H	2.5228109	-1.0642411	-2.0262211	H	3.2451775	-0.6088906	-1.3632002	H	3.8589021	0.5770134	0.0386064
H	2.2463012	0.6962016	-1.8952275	H	2.2848370	0.8947829	-1.3281839	H	2.4877221	1.7311299	0.0895677
H	3.8117845	0.0042958	-1.3648781	H	3.9060601	0.8494614	-0.5483860	H	3.7787264	1.8000216	1.3441229
C	1.8750518	1.5917744	2.9935051	C	2.3242567	1.0035378	4.0075774	C	2.0884181	-0.5689428	5.1492445
H	1.4520952	2.4971520	2.5384337	H	2.0805219	2.0641959	3.8643992	H	1.9567480	0.4442866	5.5493318
H	1.3165289	1.3323179	3.8969559	H	1.7348059	0.5923930	4.8312901	H	1.3726241	-1.2518472	5.6138955
H	1.3329124	1.2125148	-6.0023506	H	1.3208377	1.2468107	-6.0030148	H	1.0635672	0.0465492	-6.3552192

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N [⊖] +E				TS _C				N-E [⊖]			
C	-0.5700478	-0.8013658	0.9243469	C	-0.5078059	-0.8654619	0.4754579	C	-0.8189257	-0.6152851	0.3198415
C	-1.8479840	-0.3033492	0.6892167	C	-1.8466610	-0.3420935	0.4716186	C	-0.3414389	0.6381417	-0.3645472
C	-2.8454349	-1.3330626	0.3308179	C	-2.8813457	-1.3431446	0.2904113	C	-1.2550560	1.3619998	-1.1753318
C	-2.2594754	1.0975109	0.6322897	C	-2.2202058	1.0487335	0.4200282	C	1.0139253	1.0422380	-0.2376650
C	-4.5423565	0.2906512	0.9098230	C	-4.4475588	0.3182147	1.0853343	C	0.3166345	3.2055286	-1.0812262

C	0.7243753	-0.2660903	1.2691122	C	0.7356805	-0.2993239	1.0314984	C	-0.4672226	-0.6507235	1.8052265
C	1.6970222	-1.2192270	1.6704861	C	1.6306625	-1.2157210	1.6256275	C	-0.9782164	0.3824985	2.6048303
C	1.1507366	1.0834439	1.1566383	C	1.1651628	1.0431568	0.9254732	C	0.3014611	-1.6405200	2.4346003
C	3.0039459	-0.8638226	1.9774325	C	2.8799469	-0.8306568	2.1119306	C	-0.7384649	0.4463710	3.9811480
H	1.4138898	-2.2713420	1.7283996	H	1.3444411	-2.2664322	1.6977577	H	-1.5809197	1.1660368	2.1394935
C	2.4543094	1.4476502	1.4453900	C	2.4107872	1.4396370	1.3941241	C	0.5523848	-1.5963401	3.8074251
H	0.4397945	1.8298587	0.8159036	H	0.5067268	1.7665873	0.4530754	H	0.7405015	-2.4493079	1.8517126
C	3.3945465	0.4819785	1.8560342	C	3.2820264	0.5085726	1.9870335	C	0.0366333	-0.5532599	4.5911793
H	3.7125080	-1.6339566	2.2761702	H	3.5306390	-1.5782631	2.5623876	H	-1.1599856	1.2679452	4.5588074
H	2.7817351	2.4813241	1.3291095	H	2.7396028	2.4744536	1.2882048	H	1.1583926	-2.3674478	4.2867955
O	4.6553089	0.9422062	2.0862987	O	4.4933142	0.9974973	2.3961233	O	0.3409552	-0.5962470	5.9329308
C	5.6724554	-0.0148945	2.4554698	C	5.4334795	0.0690761	2.9735868	C	-0.1691453	0.4608935	6.7660508
H	5.8092332	-0.7676851	1.6640986	H	5.7009820	-0.7226395	2.2562536	H	-1.2709377	0.4785628	6.7612600
H	6.5914193	0.5677132	2.5731301	H	6.3217805	0.6624183	3.2134559	H	0.1878208	0.2380077	7.7772437
H	5.4226888	-0.5105646	3.4057197	H	5.0320443	-0.3831614	3.8939027	H	0.2169427	1.4429169	6.4484584
O	-1.5388403	2.0908095	0.6191769	O	-1.4966388	2.0308342	0.2345021	O	1.9298346	0.4064511	0.3033873
O	-2.5962422	-2.5029940	0.0571964	O	-2.7009877	-2.5308588	-0.0007207	O	-2.4129594	1.0297108	-1.4817316
O	-3.6160002	1.3414619	0.5458597	O	-3.5796333	1.3366259	0.5420338	O	1.3800587	2.2578108	-0.8346279
O	-4.1601652	-0.9426496	0.2498546	O	-4.2008714	-0.9374604	0.4049491	O	-0.7955579	2.5584332	-1.7427671
C	-5.8851356	0.6853252	0.3315671	C	-5.8634824	0.7254464	0.7284000	C	0.8660287	4.2205597	-2.0654493
H	-6.6262311	-0.0918110	0.5563152	H	-6.5699389	-0.0304398	1.0941202	H	0.0938023	4.9626553	-2.3055667
H	-6.2143353	1.6317762	0.7781880	H	-6.0997337	1.6893649	1.1965684	H	1.7297028	4.7355683	-1.6256084
H	-5.7998462	0.8049911	-0.7556917	H	-5.9596707	0.8169175	-0.3608920	H	1.1777988	3.7093347	-2.9851400
C	-4.5599260	0.0974172	2.4225147	C	-4.2266176	0.1644140	2.5886925	C	-0.1438354	3.8345524	0.2345908
H	-4.8681935	1.0330952	2.9056565	H	-4.4392734	1.1190475	3.0866958	H	0.7006594	4.3497867	0.7103971
H	-5.2746041	-0.6938492	2.6815957	H	-4.9054838	-0.6034219	2.9813020	H	-0.9423906	4.5612871	0.0365911
H	-3.5665534	-0.1847847	2.7958402	H	-3.1918202	-0.1286348	2.8068412	H	-0.5220388	3.0652137	0.9198517
H	-0.5706108	-1.8943011	0.9341371	H	-0.5369792	-1.9450255	0.6439892	H	-1.9194555	-0.5788162	0.2710067
C	0.0673064	-1.4239025	-1.7340123	C	-0.0421113	-1.2734793	-1.5521127	C	-0.4899345	-1.9709484	-0.4646643
C	-0.4453223	-0.1475880	-2.0506309	C	-0.4248007	-0.0283639	-2.1655977	C	-1.4157672	-1.9885727	-1.6577806
C	1.4407206	-1.6810986	-1.5229373	C	1.3425569	-1.6696277	-1.4910825	C	0.9583562	-2.1280855	-0.8493833
N	0.5052151	0.9117073	-2.1181543	N	0.5930085	0.9398393	-2.2816440	N	-0.9243210	-1.3606422	-2.7934031
O	-1.6577888	0.1269602	-2.2297725	O	-1.5884830	0.2499624	-2.5005337	O	-2.5543094	-2.4538466	-1.5971016
N	2.3040902	-0.5498795	-1.6395673	N	2.2792628	-0.6336029	-1.6896510	N	1.3339004	-1.4508507	-2.0035220
O	1.9320956	-2.7990049	-1.2300635	O	1.7209243	-2.8219527	-1.2096062	O	1.7724779	-2.7902861	-0.2054146
C	1.8733821	0.7345807	-1.9543607	C	1.9436381	0.6689647	-2.0693468	C	0.4135148	-0.9537409	-2.9374531
O	2.6877541	1.6645392	-2.0798941	O	2.8213518	1.5248976	-2.2238332	O	0.7624954	-0.2899976	-3.9092986
C	3.7446720	-0.7195148	-1.4440559	C	3.7037057	-0.8864802	-1.4480086	C	2.7695077	-1.2987523	-2.2767953
H	4.2848690	-0.5842024	-2.3915740	H	4.2796396	-0.7647726	-2.3741397	H	3.1877731	-2.2402781	-2.6566035
H	4.1095794	0.0187239	-0.7206737	H	4.0752839	-0.1808660	-0.6951984	H	2.8959097	-0.5081206	-3.0201844
H	3.9046340	-1.7311918	-1.0623360	H	3.7963716	-1.9107431	-1.0787692	H	3.2630447	-1.0190798	-1.3406625
C	-0.0093097	2.2546126	-2.3965023	C	0.1888054	2.2927235	-2.6783429	C	-1.8312774	-1.0222374	-3.8991014
H	0.8348514	2.9483894	-2.4106059	H	1.0531730	2.9534882	-2.5785181	H	-1.9419757	0.0670007	-3.9551942
H	-0.5232038	2.2688145	-3.3666522	H	-0.1659347	2.2970597	-3.7174749	H	-1.4313003	-1.4084051	-4.8433142
H	-0.7204361	2.5392862	-1.6111832	H	-0.6212887	2.6175943	-2.0145023	H	-2.7992824	-1.4800780	-3.6820309
H	-0.6343431	-2.2494155	-1.6492533	H	-0.7633593	-2.0833065	-1.6491992	H	-0.7690204	-2.8143473	0.1771475

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TS _{PT}				Θ _{N-E}			
C	0.0644790	-0.6965127	-0.1929152	C	0.2518596	0.0495278	-0.2833515
C	-0.3964941	-0.4445531	-1.6070892	C	-0.6739460	0.1308312	-1.4876304
C	0.5197621	-0.3703210	-2.6691616	C	-0.7868535	-0.9947870	-2.3234686
C	0.0935335	-0.2662942	-3.9916192	C	-1.6338910	-0.9995497	-3.4304338
C	-1.2795849	-0.2367053	-4.2877577	C	-2.3890764	0.1440754	-3.7373930
C	-2.2120683	-0.3140268	-3.2421378	C	-2.2829459	1.2818949	-2.9213085
C	-1.7597340	-0.4166541	-1.9205845	C	-1.4292270	1.2650899	-1.8127090
H	1.5908458	-0.3910499	-2.4617744	H	-0.2038222	-1.8913126	-2.0986141
H	0.8138977	-0.2043720	-4.8091890	H	-1.7167635	-1.8791275	-4.0712355
H	-3.2832202	-0.2908706	-3.4379972	H	-2.8533261	2.1841519	-3.1386298
H	-2.4968175	-0.4714611	-1.1174872	H	-1.3606877	2.1459629	-1.1759697
O	-1.6057772	-0.1290901	-5.6212290	O	-3.1934659	0.0524533	-4.8491542
C	-3.0031327	-0.1047988	-5.9645941	C	-3.9830129	1.2044500	-5.1995798
H	-3.5115743	0.7627304	-5.5137433	H	-3.3445034	2.0739300	-5.4237790
H	-3.0375041	-0.0213469	-7.0561596	H	-4.5390655	0.9179454	-6.0985873
H	-3.5088511	-1.0323385	-5.6510111	H	-4.6912108	1.4635239	-4.3962761
C	-0.8109778	-0.2443159	1.0050548	C	-0.4384883	-0.0525395	1.0525332
C	-1.4863837	1.0479527	1.0205190	C	-1.1035729	1.0605407	1.6205827
N	-2.1943763	1.3444312	2.2225293	N	-1.6929814	0.8553301	2.9108856
C	-2.4539492	0.4250216	3.2283175	C	-1.6169884	-0.3306573	3.6178291
N	-2.0216050	-0.8803858	3.0210217	N	-0.9191534	-1.3704043	3.0262919
C	-1.3336533	-1.3065567	1.8602686	C	-0.2814502	-1.2793671	1.7510396
O	-1.4447322	1.8877400	0.1163513	O	-1.2045238	2.1968837	1.0930846
C	-2.7550378	2.6884324	2.4114115	C	-2.4142543	1.9541632	3.5587724
O	-3.0774561	0.7420571	4.2509546	O	-2.1475221	-0.4585446	4.7375751
C	-2.4132824	-1.8674883	4.0356356	C	-0.8344982	-2.6166709	3.7935959
O	-1.1746471	-2.5205703	1.6536712	O	0.3675929	-2.2756856	1.3334367
H	-2.4271874	3.3044636	1.5702153	H	-2.3925315	2.8074588	2.8755683
H	-3.8519874	2.6477193	2.4352839	H	-3.4523187	1.6604329	3.7627345
H	-2.3933389	3.1122349	3.3560443	H	-1.9313382	2.2224904	4.5079237
H	-1.9127215	-2.8089166	3.7959220	H	-0.2741944	-3.3357396	3.1902321
H	-2.1068859	-1.5144579	5.0269724	H	-0.3172618	-2.4452580	4.7471256
H	-3.5013750	-2.0173288	4.0301632	H	-1.8406946	-3.0022925	4.0035341
H	0.5568681	0.1058937	1.3764349	H	0.8287099	2.1536898	-0.2321069
C	1.4479061	-0.1690592	0.2791439	C	1.3582113	1.1965760	-0.3064724
C	2.3597604	-1.1591607	0.8529584	C	2.2655139	1.0967346	0.8958891
O	3.6210512	-0.7179390	1.2254921	O	3.4578459	0.4461436	0.7426825
C	4.2012425	0.3643091	0.4511970	C	3.8198103	-0.2589507	-0.4791315
O	3.2548424	1.4470420	0.3114066	O	3.2253529	0.3653915	-1.6628688
C	1.9685921	1.1280288	-0.1400905	C	2.1078141	1.1470797	-1.6110985
O	1.3745225	1.9961535	-0.7620500	O	1.7633634	1.7283348	-2.6235851
O	2.0695677	-2.3177752	1.1402971	O	2.0145744	1.5844691	1.9804894
C	5.3606062	0.9017145	1.2643388	C	5.3166245	-0.0679797	-0.6369685
C	4.6072437	-0.1544637	-0.9253710	C	3.4007927	-1.7161818	-0.3781130
H	6.1035661	0.1092126	1.4189806	H	5.8338737	-0.4836447	0.2365910

H	5.8336747	1.7333985	0.7272774	H	5.6585725	-0.5917633	-1.5383371
H	4.9985160	1.2562851	2.2376699	H	5.5485636	1.0005947	-0.7258278
H	5.0471194	0.6611795	-1.5128389	H	3.5728075	-2.2103013	-1.3425138
H	5.3437429	-0.9603818	-0.8155164	H	4.0131088	-2.2090088	0.3879342
H	3.7355112	-0.5487150	-1.4659467	H	2.3479524	-1.8220074	-0.0885648
H	0.1319145	-1.7888175	-0.0676596	H	0.7879282	-0.9003721	-0.3887668

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N _O [⊖] +E				TS _O				N _O -E [⊖]			
C	1.4666371	-0.7486345	-0.6573007	C	0.8237366	-0.8820139	-1.2249612	C	-0.4348773	-0.5015484	-0.8014997
C	1.4205399	0.5315842	-0.1458476	C	1.5252281	0.1396150	-0.5011507	C	0.9708926	-0.3249168	-0.3234329
C	0.7161703	0.9392247	1.0824024	C	1.0930705	0.5925606	0.7994346	C	1.2695357	-0.3280844	1.0663830
C	1.9367576	1.5928678	-1.0460986	C	2.4769842	0.9299156	-1.2430773	C	1.9750922	-0.0608074	-1.2954756
C	1.8635568	3.0784853	0.8763487	C	3.2114442	1.7719988	0.9111089	C	3.5794013	-0.6745948	0.4149993
C	1.1119080	-2.0517309	-0.1586356	C	0.3808412	-2.1620336	-0.6088676	C	-1.0277909	-1.8648438	-0.5257538
C	0.9592586	-2.4188469	1.2035058	C	0.7938754	-2.5760031	0.6711502	C	-1.6229496	-2.1984817	0.7032543
C	0.9153339	-3.0626672	-1.1320055	C	-0.4210207	-3.0435523	-1.3531616	C	-0.9285967	-2.8549341	-1.5098938
C	0.5925119	-3.7048460	1.5580544	C	0.3907494	-3.7981559	1.1989093	C	-2.0971873	-3.4866311	0.9374085
H	1.1344915	-1.6850586	1.9843153	H	1.4486447	-1.9384226	1.2625929	H	-1.6996733	-1.4378166	1.4775668
C	0.5175128	-4.3500360	-0.7924309	C	-0.8468797	-4.2687064	-0.8370581	C	-1.3909612	-4.1579210	-1.2873038
H	1.0371808	-2.8073630	-2.1858569	H	-0.7487726	-2.7489281	-2.3507301	H	-0.4745695	-2.6144986	-2.4742738
C	0.3458378	-4.6781550	0.5657498	C	-0.4452396	-4.6491903	0.4548063	C	-1.9800363	-4.4771664	-0.0540705
H	0.4844164	-3.9868523	2.6062571	H	0.7171497	-4.1132210	2.1913271	H	-2.5634939	-3.7466110	1.8894397
H	0.3492485	-5.0850921	-1.5773919	H	-1.4810498	-4.9129577	-1.4440924	H	-1.2954354	-4.9005579	-2.0779685
H	1.8366149	-0.7670829	-1.6859784	H	1.2496377	-1.0213008	-2.2212021	H	-0.4480354	-0.3231882	-1.8867177
O	2.3332553	1.4221737	-2.1928738	O	2.7042524	0.8713902	-2.4569032	O	1.8115942	0.1731546	-2.5059135
O	-0.0079500	0.2339558	1.7699263	O	0.0774288	0.2486303	1.4055166	O	0.4708637	-0.3269684	2.0142357
O	1.9575488	2.8710136	-0.5581040	O	3.1904430	1.8867952	-0.5349922	O	3.2986560	-0.0136302	-0.8445091
O	0.8035232	2.2630839	1.4339587	O	1.8670676	1.5769979	1.4080312	O	2.6289976	-0.2487982	1.4175411
C	1.4284690	4.5149321	1.0669182	C	3.6681485	3.1189430	1.4354197	C	4.9367216	-0.1710111	0.8668989
H	1.3281751	4.7275844	2.1386980	H	3.6830339	3.1031231	2.5325458	H	5.1978980	-0.6238708	1.8318875
H	2.1812580	5.1881530	0.6377037	H	4.6789941	3.3370734	1.0683429	H	5.6999187	-0.4451556	0.1273587
H	0.4626108	4.6580431	0.5649949	H	2.9795896	3.9014384	1.0924415	H	4.9107293	0.9210118	0.9737553
C	3.1917133	2.7269949	1.5354163	C	4.1157108	0.6188349	1.3412847	C	3.5330295	-2.1931918	0.2408200
H	3.9853984	3.3627309	1.1233721	H	5.1359143	0.7981437	0.9785672	H	4.2741233	-2.4984417	-0.5092009
H	3.1191187	2.8962962	2.6171134	H	4.1304025	0.5572130	2.4370038	H	3.7712408	-2.6772918	1.1968037
H	3.4509153	1.6741640	1.3572073	H	3.7554679	-0.3349462	0.9350650	H	2.5377499	-2.5200549	-0.0862769
O	-0.0383464	-5.8994183	1.0212453	O	-0.8007748	-5.8231244	1.0658078	O	-2.4754074	-5.7158506	0.2757230
C	-0.3114900	-6.9371741	0.0523550	C	-1.6556083	-6.7281437	0.3389341	C	-2.3753895	-6.7603685	-0.7106215
H	-0.6094983	-7.8110004	0.6398985	H	-1.8153746	-7.5808333	1.0070062	H	-2.8176824	-7.6477513	-0.2456065
H	-1.1326693	-6.6422468	-0.6181382	H	-2.6233510	-6.2582372	0.1028685	H	-2.9378478	-6.5041729	-1.6226793
H	0.5885927	-7.1735291	-0.5347590	H	-1.1732198	-7.0725322	-0.5893336	H	-1.3244165	-6.9659131	-0.9696129
O	-0.7875066	-0.4140133	-2.6237079	O	-0.7205292	-0.2388156	-1.8894424	O	-1.3820006	0.4745482	-0.1720117
C	-1.2477219	0.3984050	-1.7809043	C	-1.1723721	0.8391593	-1.3031547	C	-1.1124724	1.7771665	-0.2505108
N	-2.0185135	-0.1057328	-0.6856793	N	-2.2385993	0.6785515	-0.4076622	N	-1.7140700	2.4908810	0.7718080
C	-1.0533327	1.7942548	-1.7986518	C	-0.6404757	2.0958119	-1.5053495	C	-0.3594157	2.4037015	-1.2109843

C	-2.5271978	0.6900623	0.3284494	C	-2.7002720	1.7247590	0.3812775	C	-1.6325820	3.8850227	0.8387986
C	-1.5295643	2.6689061	-0.7995416	C	-1.0943728	3.2367170	-0.7809291	C	-0.1943246	3.8215104	-1.1973554
H	-0.4606501	2.2153561	-2.6064762	H	0.1782662	2.2155275	-2.2088828	H	0.1338664	1.8387186	-1.9973442
N	-2.2461644	2.0470192	0.2714421	N	-2.1389944	2.9787213	0.1503994	N	-0.8748632	4.5050543	-0.1466149
O	-3.2068848	0.2084093	1.2521574	O	-3.5762718	1.5646050	1.2448368	O	-2.1934710	4.5328363	1.7311830
O	-1.3648864	3.9158846	-0.7795325	O	-0.6389048	4.3928582	-0.9062528	O	0.4726216	4.4667057	-2.0297430
C	-2.2458362	-1.5452688	-0.5575502	C	-2.7132543	-0.6750184	-0.0946478	C	-2.4108406	1.7592578	1.8437846
H	-1.7698069	-2.0265487	-1.4156162	H	-2.6771734	-1.2795926	-1.0041830	H	-3.3331093	1.3064240	1.4592661
H	-1.7868566	-1.9150040	0.3689463	H	-2.0542579	-1.1280465	0.6586879	H	-1.7444115	0.9742817	2.2206037
H	-3.3212168	-1.7661046	-0.5413868	H	-3.7363157	-0.6095585	0.2847098	H	-2.6520148	2.4750601	2.6328267
C	-2.6729028	2.8487352	1.4175980	C	-2.6582622	4.0769736	0.9723335	C	-0.7852496	5.9681111	-0.0621525
H	-3.7646581	2.8167214	1.5317687	H	-3.7434337	4.1659013	0.8377365	H	-1.7876441	6.4097623	-0.1245746
H	-2.2052109	2.4621042	2.3326723	H	-2.4468608	3.8907035	2.0333842	H	-0.3236606	6.2631970	0.8885712
H	-2.3436016	3.8752578	1.2349240	H	-2.1606747	4.9947968	0.6482233	H	-0.1709931	6.3090092	-0.8994770

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C	-0.4952222	-1.5038760	-0.4628462	C	-0.4825544	-0.9649688	0.4685692	C	-0.6272188	0.8233216	0.3637362
C	-1.7545340	-1.1693306	0.0294989	C	-1.8138304	-0.4241945	0.6726112	C	0.5086152	0.4779217	-0.5607393
C	-2.8214805	-1.1831052	-0.9874308	C	-2.8668243	-1.4049576	0.5332237	C	0.9034148	1.4484388	-1.5198672
C	-2.0703572	-0.7456923	1.3855380	C	-2.1345909	0.9683722	0.7968726	N	2.1344921	-1.0788297	-1.4525026
C	-4.3054448	-0.0078297	0.5896456	C	-4.5514066	0.3718471	0.8966984	N	1.9254327	1.0560193	-2.4366167
N	-4.0650077	-0.6509270	-0.6189426	N	-4.2008504	-0.9532975	0.6904482	C	2.5317577	-0.1891135	-2.4341456
N	-3.3312931	-0.1400276	1.5735343	N	-3.5183185	1.2872848	0.9642887	O	3.3998840	-0.4903111	-3.2740431
C	-5.0847594	-0.5540531	-1.6704567	C	-5.3097799	-1.9103405	0.5974243	C	2.7760779	-2.3954930	-1.4656246
H	-6.0336528	-0.2709426	-1.2094259	H	-5.9226063	-1.8620665	1.5060393	H	2.5905642	-2.9029154	-2.4218958
H	-4.7887857	0.2025846	-2.4102765	H	-5.9424413	-1.6777792	-0.2693799	H	3.8603214	-2.2938478	-1.3268577
H	-5.1776630	-1.5240480	-2.1696121	H	-4.8778495	-2.9076676	0.4848996	H	2.3438878	-2.9755352	-0.6454636
C	-3.6592412	0.4446218	2.8808180	C	-3.9126261	2.6893464	1.1411830	C	2.3449830	1.9821208	-3.4918338
H	-3.8560198	1.5179666	2.7685147	H	-4.4990371	3.0343992	0.2789272	C	1.1026211	-0.8090158	-0.4957828
H	-4.5503013	-0.0389869	3.3000097	H	-4.5209589	2.7953727	2.0478659	H	3.4232841	2.1757736	-3.4235825
H	-2.8025727	0.2861383	3.5394676	H	-2.9976212	3.2802744	1.2257351	H	2.1253578	1.5579118	-4.4807856
O	-5.3529802	0.6082536	0.8142615	O	-5.7397020	0.7167405	1.0079996	H	1.7863138	2.9113684	-3.3518589
C	0.8568798	-1.4868947	-0.0044575	C	0.8324053	-0.5107198	0.9623915	C	-0.3478105	0.5296169	1.8339977
C	1.8407806	-1.9134476	-0.9465832	C	1.7450034	-1.5247676	1.3406071	C	-1.2145886	-0.1326019	2.7099099
C	1.3505731	-0.9831478	1.2304864	C	1.3387404	0.8064213	0.9476989	C	0.8446286	1.0314162	2.3821840
C	3.1936405	-1.8508800	-0.6924228	C	3.0608519	-1.2572886	1.6932519	C	-0.9111101	-0.2977730	4.0653540
H	1.5093581	-2.2755298	-1.9219347	H	1.4116613	-2.5648595	1.3326277	H	-2.1473389	-0.5607771	2.3436067
C	2.7014863	-0.9027330	1.4968116	C	2.6566631	1.0920681	1.2819854	C	1.1666530	0.8797039	3.7291115
H	0.6384074	-0.6443755	1.9769348	H	0.6746020	1.6101792	0.6435519	H	1.5451885	1.5591088	1.7299268
C	3.6750804	-1.3192047	0.5404756	C	3.5656203	0.0701247	1.6651759	C	0.2988871	0.1896528	4.6150754
H	3.8892323	-2.1692372	-1.4660995	H	3.7072936	-2.0907970	1.9624621	H	-1.6301042	-0.8232684	4.6922689
H	3.0163760	-0.4751539	2.4463461	H	2.9904449	2.1257951	1.2131348	H	2.1034281	1.3027758	4.0892709
C	5.9878811	-1.5193470	-0.2526264	C	5.8342920	-0.7449144	2.1260241	N	0.6336155	-0.0158954	5.9548855
H	5.8764703	-0.8701963	-1.1371361	H	5.9655342	-1.3090863	1.1841718	C	-0.4214924	-0.4332479	6.8756500
H	6.9947531	-1.3837578	0.1529793	H	6.8048361	-0.3337460	2.4235477	H	-0.8560026	-1.3938699	6.5649000
H	5.8855035	-2.5672792	-0.5712077	H	5.5151545	-1.4482074	2.9086880	H	0.0138442	-0.5749157	7.8715109

N	5.0107524	-1.1857992	0.7837446	N	4.8791343	0.3520550	1.9873361	H	-1.2401651	0.3088329	6.9515374
C	5.4780325	-0.5193936	1.9998533	C	5.4186296	1.6778566	1.6927279	C	1.7021982	0.7945767	6.5359064
H	5.1386658	0.5290781	2.0425900	H	5.4033838	1.9054696	0.6108996	H	1.4744876	1.8781861	6.5175743
H	5.1200658	-1.0401550	2.9004235	H	4.8513156	2.4595785	2.2181958	H	1.8516737	0.4877215	7.5774463
H	6.5717997	-0.5306755	2.0115111	H	6.4548243	1.7244147	2.0443571	H	2.6509087	0.6331421	6.0050264
O	-1.3213046	-0.8842569	2.3666033	O	-1.3222103	1.9159474	0.7824892	O	0.7682981	-1.7126232	0.3027982
O	-2.6849988	-1.6274755	-2.1379705	O	-2.6737529	-2.6165785	0.2797868	O	0.4029636	2.5958221	-1.6319435
H	-0.5681611	-1.8290188	-1.5050536	H	-0.5417876	-2.0542648	0.5494990	H	-0.7488926	1.9164651	0.2829039
C	-0.2184333	1.1715385	-2.0884258	C	-0.2963448	-1.1336282	-1.5558994	C	-2.0472125	0.2866928	-0.1509063
C	-0.9169999	1.6232418	-0.9523866	C	-0.6857739	0.1849315	-2.0016366	C	-2.3865857	1.0999587	-1.3774349
C	1.1882010	1.1161026	-2.1735212	C	1.0658203	-1.5861506	-1.7471495	C	-2.0660786	-1.1989908	-0.4036609
N	-0.1031359	1.9765851	0.1739264	N	0.3552074	1.1244962	-2.1203406	N	-1.8574298	0.6093467	-2.5622998
O	-2.1668340	1.7107801	-0.8472522	O	-1.8637677	0.5346786	-2.1787293	O	-3.0153137	2.1574332	-1.3162265
N	1.8994159	1.5625645	-1.0145693	N	2.0202681	-0.5693543	-1.9402580	N	-1.5327820	-1.5753283	-1.6352540
O	1.8477619	0.7242992	-3.1708018	O	1.4109773	-2.7786860	-1.6717735	O	-2.5020713	-2.0207553	0.4019731
C	1.2825433	2.0167774	0.1429068	C	1.7069120	0.7836041	-2.1087304	C	-1.2631720	-0.6613697	-2.6623833
O	1.9382586	2.4447713	1.1093507	O	2.6006460	1.6209016	-2.2655781	O	-0.6502314	-0.9960918	-3.6726426
C	3.3609815	1.6057125	-1.0497249	C	3.4497606	-0.8970378	-1.9081496	C	-1.1592516	-2.9724852	-1.8859367
H	3.7215591	2.6166744	-1.2930032	H	3.9194385	-0.6708334	-2.8736805	H	-1.7166894	-3.3676582	-2.7440048
H	3.7530972	1.3141228	-0.0707551	H	3.9350623	-0.3095774	-1.1192781	H	-0.0836356	-3.0288355	-2.0872807
H	3.6961060	0.9025422	-1.8170675	H	3.5367203	-1.9635036	-1.6868099	H	-1.3973230	-3.5425493	-0.9850110
C	-0.7430036	2.3906937	1.4225976	C	-0.0279456	2.5312474	-2.2788137	C	-1.7967632	1.4575943	-3.7593412
H	-0.4192110	1.7385898	2.2439279	H	0.8730098	3.1441114	-2.1980424	H	-0.7513585	1.7102574	-3.9732048
H	-0.4897215	3.4308323	1.6679752	H	-0.5026455	2.6927415	-3.2555351	H	-2.2355459	0.9317795	-4.6148527
H	-1.8224091	2.2921046	1.2759118	H	-0.7367350	2.7824313	-1.4796998	H	-2.3591947	2.3696640	-3.5451482
H	-0.8026561	0.8365020	-2.9419473	H	-1.0560385	-1.9036844	-1.6876007	H	-2.8003088	0.5179141	0.6100898

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C	-0.0955015	0.7612613	0.0124239	C	0.9458613	0.3982681	0.0875969
C	0.8152681	0.2763572	1.1743926	C	1.3596962	-0.0010865	1.4814455
C	1.6064983	1.3114953	1.8409178	C	0.7668914	-1.0790185	2.1906116
N	1.5545605	-1.3099696	2.8658106	N	2.9206350	0.3419728	3.3165817
N	2.5050370	0.8601465	2.8353501	N	1.2922542	-1.3480923	3.4993112
C	3.4658125	1.7997129	3.4287526	C	0.7066531	-2.4273254	4.2992185
H	3.2503309	1.9445834	4.4953870	H	1.4676576	-3.1823752	4.5371460
H	4.4837436	1.4060957	3.3211411	H	0.3004353	-2.0292977	5.2386332
H	3.3700328	2.7508411	2.8993598	H	-0.0920923	-2.8768217	3.7035914
C	1.5023569	-2.6324779	3.5015033	C	4.0474419	1.0519675	3.9297147
H	2.4949561	-3.0960021	3.4654281	H	3.7325569	1.5234644	4.8698777
H	1.1853753	-2.5482941	4.5500004	H	4.8680531	0.3543090	4.1439054
H	0.7789121	-3.2378447	2.9493128	H	4.3810931	1.8135822	3.2202690
C	0.5607285	-0.9649254	1.9001555	C	2.4870576	0.7001704	2.0032258
C	2.5189796	-0.4357220	3.3417850	C	2.3433649	-0.6614680	4.0746237
O	3.3366895	-0.7770586	4.2080195	O	2.7581159	-0.9351628	5.2169417
O	-0.3968147	-1.7221046	1.7246340	O	3.1210856	1.6057572	1.3995725
O	1.5787317	2.5163683	1.5407145	O	-0.1630695	-1.8128149	1.7767007

C	-1.5841404	0.5279226	0.0444217	C	-0.4862656	0.8081682	-0.2101933
C	-2.3054697	0.6160621	1.2432422	C	-0.6891593	2.0508646	-0.8392075
C	-2.3224338	0.3465704	-1.1311748	C	-1.6270622	0.0070966	-0.0262159
C	-3.6971428	0.5276328	1.2767121	C	-1.9419357	2.4751253	-1.2785927
H	-1.7660448	0.7406500	2.1846967	H	0.1683654	2.7076552	-1.0067286
C	-3.7163272	0.2551465	-1.1230362	C	-2.8873853	0.4081968	-0.4652282
H	-1.7995228	0.2614405	-2.0861295	H	-1.5089822	-0.9549757	0.4681758
C	-4.4492649	0.3601889	0.0854859	C	-3.0820947	1.6446624	-1.1329664
H	-4.1974512	0.5877820	2.2421473	H	-2.0233065	3.4518471	-1.7529628
H	-4.2305879	0.0989416	-2.0701742	H	-3.7268851	-0.2651041	-0.2996130
C	-6.5182094	0.0868667	1.3777012	C	-4.5300805	3.3962535	-2.0609514
H	-6.2744351	0.8776807	2.1010273	H	-3.8264271	3.6722998	-2.8595808
H	-7.6020072	0.1117327	1.2158872	H	-5.5439145	3.4937080	-2.4650150
H	-6.2519127	-0.8891809	1.8283574	H	-4.4121426	4.1185208	-1.2306112
N	-5.8459954	0.3210167	0.1014049	N	-4.3218409	2.0145626	-1.6367325
C	-6.5374711	-0.1837404	-1.0828268	C	-5.5058412	1.2654694	-1.2247603
H	-6.2761781	-1.2347664	-1.3149201	H	-5.6902592	1.3269530	-0.1352052
H	-7.6187041	-0.1227552	-0.9137242	H	-6.3797004	1.6686438	-1.7486240
H	-6.3058838	0.4306699	-1.9643236	H	-5.4143853	0.2046492	-1.4991070
H	0.0579630	1.8519272	-0.0050767	H	1.5486049	1.2939687	-0.1178127
C	0.7426493	0.2579789	-1.1870810	C	1.5522722	-0.6104566	-1.0378313
C	0.5819806	-1.0919813	-1.7085007	C	1.2287131	-2.0461881	-0.7727357
C	1.3359906	1.2803649	-2.0399746	C	1.0813325	-0.1076559	-2.3707798
N	1.4047034	-1.4209270	-2.8254310	N	0.0109842	-2.4950377	-1.2834863
O	-0.1536928	-1.9557827	-1.2182867	O	1.9663173	-2.7878958	-0.1262761
N	2.1506750	0.8118601	-3.0992029	N	-0.0873191	-0.6905435	-2.8544482
O	1.2084976	2.5046428	-1.8651094	O	1.6340731	0.8292988	-2.9501004
C	2.2000743	-0.5147806	-3.5110405	C	-0.6806647	-1.8395747	-2.3046615
O	2.9049721	-0.8665294	-4.4677988	O	-1.7372472	-2.2727389	-2.7587830
C	2.9272507	1.7708902	-3.8957148	C	-0.8316812	-0.0428140	-3.9443811
H	3.9667845	1.4308420	-3.9680897	H	-0.9504746	-0.7320944	-4.7882453
H	2.5097789	1.8605825	-4.9076526	H	-1.8181370	0.2585719	-3.5709352
H	2.8780797	2.7393141	-3.3917533	H	-0.2633046	0.8372844	-4.2541848
C	1.4180153	-2.8015074	-3.3252266	C	-0.5128547	-3.7715839	-0.7811704
H	1.0508722	-2.8365217	-4.3589942	H	-1.5872651	-3.8061855	-0.9790844
H	2.4395663	-3.2006652	-3.2963096	H	-0.0178796	-4.6175807	-1.2766461
H	0.7643077	-3.3921038	-2.6783705	H	-0.3216503	-3.8001377	0.2963619
H	1.5674017	-0.0249119	-0.0160395	H	2.6402082	-0.4936976	-0.9800043

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C	-1.4928076	-0.1551949	-0.5062754	C	-0.1371268	-1.0094309	-0.7853985	C	0.1315228	-0.7994583	-0.5829781
C	-1.4066846	0.3306529	0.7936456	C	-1.1313867	-0.3741408	0.0727474	C	-1.1224670	-0.2971245	0.0421829
C	-0.7945825	1.5888358	1.2100242	C	-1.1406124	1.0464323	0.2418813	C	-1.3702132	1.1019184	0.0857314
C	-2.0216941	-0.5567872	1.8080897	C	-1.9277953	-1.2403414	0.8883710	C	-1.9785569	-1.2468961	0.6607105
C	-1.2749060	1.0003171	3.5760337	C	-2.8677528	0.7622071	2.0114612	C	-3.4531730	0.6238708	1.3631327
C	-1.0173031	0.1814666	-1.8089009	C	-0.0065724	-0.6832234	-2.2289001	C	0.3217237	-0.5808158	-2.0656930

C	-0.0833709	1.1950477	-2.1667119	C	-0.8862749	0.1828512	-2.8966465	C	-0.7140248	-0.1266216	-2.8900946
C	-1.4559184	-0.6708725	-2.8689315	C	0.9923844	-1.3071367	-2.9990688	C	1.5465602	-0.8929431	-2.6770793
C	0.3606185	1.3494836	-3.4636723	C	-0.7754056	0.4303171	-4.2621406	C	-0.5455872	0.0189173	-4.2672117
H	0.2986330	1.8453939	-1.3865679	H	-1.6810741	0.6739110	-2.3354673	H	-1.6771670	0.1256157	-2.4431003
C	-1.0336078	-0.5211168	-4.1721287	C	1.1320167	-1.0637658	-4.3614070	C	1.7402772	-0.7473794	-4.0492526
H	-2.1498315	-1.4816591	-2.6351797	H	1.6956484	-1.9846883	-2.5098936	H	2.3791341	-1.2404903	-2.0618539
C	-0.0998402	0.5030094	-4.5186165	C	0.2401563	-0.1883611	-5.0413071	C	0.6883068	-0.2991313	-4.8929115
H	1.0916934	2.1289281	-3.6705173	H	-1.4865016	1.1122046	-4.7256923	H	-1.3844413	0.3862757	-4.8562326
H	-1.4062836	-1.2086043	-4.9290015	H	1.9360113	-1.5611880	-4.9014151	H	2.7170865	-0.9888498	-4.4653584
H	-2.0722578	-1.0847860	-0.5169665	H	-0.1287126	-2.0915068	-0.6146703	H	0.2159207	-1.8756719	-0.3673838
O	-2.6698101	-1.5766077	1.5317797	O	-1.9167905	-2.4930028	0.8301585	O	-1.7864007	-2.4898041	0.6837668
O	-0.3343607	2.4408200	0.4336410	O	-0.4140718	1.8541138	-0.3732048	O	-0.6307886	1.9869574	-0.4018239
C	1.3313517	1.6854576	-6.1244280	C	-0.4344704	1.1068852	-7.0150768	C	-0.1450844	0.5294603	-7.0476417
H	2.2809702	1.5077039	-5.5950265	H	-0.1682283	2.1025323	-6.6146262	H	-0.2236244	1.5933744	-6.7536770
H	1.5256523	1.6589068	-7.2004217	H	-0.2495919	1.1053356	-8.0945705	H	0.1295545	0.4803973	-8.1071361
H	0.9656728	2.6906880	-5.8648938	H	-1.5121336	0.9495200	-6.8607136	H	-1.1373033	0.0679709	-6.9400641
N	-0.7725394	1.8504319	2.5944681	N	-2.0465841	1.5526798	1.2256125	N	-2.5695355	1.5028528	0.7616299
N	-1.8450122	-0.1927678	3.1507159	N	-2.7992151	-0.6094208	1.8181702	N	-3.1429733	-0.7252438	1.2996288
O	-1.2496651	1.3124271	4.7686545	O	-3.6325665	1.2585106	2.8558244	O	-4.4813582	1.0259937	1.9377956
C	-0.2002151	3.1116363	3.0831518	C	-2.1111567	2.9975715	1.4668808	C	-2.9053557	2.9265998	0.8499164
H	0.2313393	3.6369898	2.2287524	H	-1.3924267	3.4724059	0.7939416	H	-2.1165269	3.4801971	0.3333911
H	-0.9817840	3.7274265	3.5464570	H	-3.1230653	3.3725631	1.2653944	H	-3.8753435	3.1201603	0.3733299
H	0.5747275	2.8966568	3.8275414	H	-1.8526401	3.2205899	2.5101426	H	-2.9592788	3.2422914	1.9002072
C	-2.2546542	-1.1189068	4.2128481	C	-3.6704776	-1.4283402	2.6678850	C	-4.0860628	-1.6405653	1.9493639
H	-2.5870818	-2.0444984	3.7376359	H	-3.5308604	-2.4714865	2.3734118	H	-3.7061613	-2.6559157	1.8094035
H	-1.3916059	-1.3099440	4.8618879	H	-3.4019282	-1.3002913	3.7247598	H	-4.1610420	-1.4130575	3.0208625
H	-3.0715189	-0.6899018	4.8067115	H	-4.7181533	-1.1322403	2.5307300	H	-5.0822341	-1.5445283	1.4979437
N	0.3379548	0.6606215	-5.7981280	N	0.3448032	0.0347120	-6.4012320	N	0.8553540	-0.1946160	-6.2672316
C	-0.1236608	-0.2371931	-6.8581994	C	1.5267557	-0.4366077	-7.1187324	C	2.2048987	-0.2567499	-6.8236493
H	0.3194965	0.0786802	-7.8069188	H	1.4116409	-0.2023392	-8.1824035	H	2.1402480	-0.1918490	-7.9154233
H	0.1784720	-1.2786698	-6.6632453	H	2.4569722	0.0371077	-6.7541820	H	2.8517866	0.5643597	-6.4606215
H	-1.2190487	-0.2010891	-6.9604373	H	1.6352945	-1.5273014	-7.0271492	H	2.6890505	-1.2124603	-6.5765082
O	0.1954011	-3.5003910	0.2201934	O	1.4329246	-0.6055396	-0.2107620	O	1.3457254	-0.1467041	0.0526355
H	2.1086967	2.0449961	1.3054200	H	1.9632410	1.1258313	5.4829886	H	2.1548249	0.8098199	5.8988697
C	0.7218501	-2.4557326	0.6828036	C	1.5805547	-0.5374792	1.0936775	C	1.5072889	-0.2551454	1.3678324
N	1.4212466	-1.5859891	-0.2175438	N	2.3284467	0.5589552	1.5227802	N	2.2781534	0.7770242	1.8793774
C	0.6978976	-2.0471247	2.0308075	C	1.0669824	-1.4231959	2.0177563	C	1.0135973	-1.2432578	2.1846589
C	2.0437456	-0.4104580	0.1727846	C	2.6127646	0.7839946	2.8695722	C	2.6428201	0.8237962	3.2274066
C	1.2725492	-0.8512744	2.4999133	C	1.2692956	-1.2463761	3.4149284	C	1.3028848	-1.2491675	3.5811892
H	0.1521443	-2.6627018	2.7416299	H	0.4625376	-2.2644394	1.6910912	H	0.3742001	-2.0299817	1.7938972
N	1.9163061	-0.0420401	1.5034084	N	2.0638514	-0.1151181	3.7753771	N	2.1426492	-0.1884848	4.0358780
O	2.6877992	0.2872639	-0.6315156	O	3.3047180	1.7407499	3.2480875	O	3.3615159	1.7233374	3.6816329
O	1.2473359	-0.4390682	3.6883859	O	0.8238682	-1.9994420	4.3058525	O	0.8919155	-2.1051753	4.3895713
C	1.5561038	-1.9708383	-1.6230497	C	2.7883665	1.5321955	0.5201317	C	2.6759129	1.8820453	0.9899420
H	0.7807328	-2.7100905	-1.8401856	H	3.5811707	1.0950470	-0.1002886	H	3.4643406	1.5538056	0.3007887
H	1.4251818	-1.0884216	-2.2570927	H	1.9324616	1.8054846	-0.1081769	H	1.7966435	2.1993692	0.4165348
H	2.5468483	-2.4093116	-1.8164722	H	3.1766220	2.4041159	1.0519881	H	3.0497400	2.6959766	1.6154948

C	2.5407620	1.2226415	1.8902242	C	2.3509165	0.1415456	5.1912282	C	2.5194156	-0.1243282	5.4532409
H	2.3355641	1.3699693	2.9541202	H	1.8600334	-0.6430254	5.7730365	H	2.0629893	-0.9820874	5.9538869
H	3.6249129	1.1912264	1.7159572	H	3.4340008	0.1198770	5.3671922	H	3.6112358	-0.1651476	5.5540269

B + 5a											
$N^{\ominus}+E$				TS_c				$N-E^{\ominus}$			
C	-1.6299724	-1.2855461	1.2142309	C	-1.9926792	-1.3992063	0.9283856	C	-2.2168540	-1.4251964	0.7578369
N	-0.2927406	-1.4907303	1.4848465	N	-0.7615356	-1.4799169	1.5567498	N	-1.0583123	-1.4923513	1.5187580
C	0.7193112	-1.8074572	0.5390933	C	0.4863444	-1.6316205	0.9291693	C	0.2490189	-1.5649348	1.0448297
C	0.2919156	-1.8681908	-0.8089841	C	0.4706069	-1.5371394	-0.5177063	C	0.4264966	-1.3654375	-0.4319228
C	-1.0599893	-1.6665157	-1.1890840	C	-0.7868766	-1.6476469	-1.2356567	C	-0.8005206	-1.5810743	-1.2749229
N	-1.9521216	-1.3812295	-0.1236794	N	-1.9398044	-1.4929551	-0.4528057	N	-2.0185518	-1.4839113	-0.6165740
O	-2.4680130	-1.0398786	2.0943137	O	-3.0515920	-1.2717432	1.5473939	O	-3.3350174	-1.3506149	1.2595748
O	1.8912795	-1.9534455	0.9601860	O	1.5135555	-1.7449889	1.6138610	O	1.1898064	-1.7253838	1.8179192
O	-1.5243028	-1.6933017	-2.3529235	O	-0.8909385	-1.7809494	-2.4657767	O	-0.7509811	-1.7416544	-2.4938744
H	1.0229394	-2.1037116	-1.5778078	H	1.3303626	-1.9807737	-1.0175629	H	1.2168043	-2.0414187	-0.7808743
H	-0.0104606	-1.4329380	2.4618565	H	-0.7738590	-1.4546889	2.5760908	H	-1.1934579	-1.5370266	2.5296459
H	-2.9201810	-1.1856306	-0.3724496	H	-2.8350906	-1.4620160	-0.9397190	H	-2.8654954	-1.5179253	-1.1856819
C	1.1018993	0.8643994	-0.9220881	C	1.0281235	0.4149203	-0.8673214	C	0.9755317	0.1382768	-0.7760648
C	2.2525180	0.8060567	-0.1556040	C	2.2935637	0.6447099	-0.2273642	C	2.3282018	0.4110197	-0.1685727
C	3.4373912	0.2701183	-0.7353491	C	3.4429939	0.0525327	-0.7874996	C	3.4187334	-0.2977001	-0.6740869
N	4.4108922	-0.1558658	-1.2220924	N	4.3842869	-0.4534928	-1.2755307	N	4.3110422	-0.9195639	-1.1346316
C	2.3780820	1.1982107	1.2043668	C	2.4837016	1.3425738	0.9798399	C	2.5467619	1.2352579	0.9336299
N	2.5315052	1.5353188	2.3134768	N	2.6839008	1.9508777	1.9651521	N	2.7550073	1.9501394	1.8502976
C	-0.2164763	1.3721016	-0.6016781	C	-0.1895510	1.2026646	-0.5648765	C	-0.0983477	1.1734761	-0.5112570
C	-0.6526964	1.7099594	0.7005078	C	-0.5760439	1.5589919	0.7418059	C	-0.4934299	1.5380510	0.7874407
C	-1.1383581	1.4839965	-1.6708062	C	-1.0401906	1.5462090	-1.6349218	C	-0.7728880	1.7452836	-1.6028648
C	-1.9568397	2.1471189	0.9167013	C	-1.7717361	2.2437575	0.9669988	C	-1.5361805	2.4472491	0.9869562
H	0.0163286	1.6058486	1.5516798	H	0.0444493	1.2803117	1.5916935	H	0.0125739	1.1129020	1.6536077
C	-2.4398577	1.9272912	-1.4492350	C	-2.2325515	2.2364955	-1.4087064	C	-1.8140390	2.6579788	-1.4063012
H	-0.8240543	1.2006821	-2.6762357	H	-0.7622403	1.2584728	-2.6505174	H	-0.4821040	1.4642976	-2.6174805
C	-2.8549630	2.2575406	-0.1534004	C	-2.6042321	2.5852558	-0.1052189	C	-2.2012137	3.0095666	-0.1086115
H	-2.2821936	2.3873419	1.9293866	H	-2.0596102	2.5017571	1.9873600	H	-1.8306812	2.7149869	2.0032021
H	-3.1368767	2.0021456	-2.2850031	H	-2.8766062	2.4947975	-2.2510092	H	-2.3256096	3.0902976	-2.2681610
H	-3.8775894	2.5939983	0.0247873	H	-3.5402996	3.1165350	0.0751922	H	-3.0169477	3.7174376	0.0488167
H	1.2319090	0.5525459	-1.9596382	H	1.1258578	0.1904751	-1.9325904	H	1.1019414	0.0656298	-1.8663189

B + 5a											
TS_{PT}				${}^{\ominus}N-E$							
C	-0.5743559	0.5036170	0.5743038	C	0.3993412	0.2259194	-3.3126346				
C	-0.4521653	-0.6174429	1.5791361	N	0.8474997	-0.9109060	-2.6778669				
C	-0.2242917	-0.3486687	2.9370642	C	0.6649320	-1.2452382	-1.3102056				
C	-0.1926537	-1.3874257	3.8744753	C	-0.0444956	-0.2909959	-0.5246933				
C	-0.3910446	-2.7109909	3.4657956	C	-0.5409444	0.9055949	-1.1008781				
C	-0.6251307	-2.9868061	2.1127549	N	-0.2890612	1.0850741	-2.4851690				

C	-0.6539378	-1.9474643	1.1786216	O	0.5962200	0.4550989	-4.5173724
H	-0.0706679	0.6795165	3.2698201	O	1.1410915	-2.3359631	-0.9118190
H	-0.0106563	-1.1599475	4.9265479	O	-1.1927137	1.8148248	-0.5159653
H	-0.3635083	-3.5220148	4.1956705	C	-0.2511208	-0.6241544	0.9326949
H	-0.7807828	-4.0155356	1.7821432	C	-1.7478117	-0.3488038	1.3624046
H	-0.8314104	-2.1723759	0.1249327	C	-2.6757122	-1.1112052	0.5256108
C	-0.2006913	0.2403664	-0.8952041	N	-3.3935385	-1.7207853	-0.1569405
C	-1.2723781	0.2704123	-1.8838184	C	-1.9735206	-0.6394458	2.7773110
N	-0.8964653	-0.0776548	-3.1917933	N	-2.1224618	-0.8680771	3.9081146
C	0.3129770	-0.6225782	-3.5860829	C	0.7120225	0.0678252	1.8876818
N	1.2214672	-0.7978026	-2.5587375	C	1.6088595	-0.7092380	2.6365243
C	1.0320224	-0.4776860	-1.2012388	C	0.7345720	1.4654775	2.0381514
O	-2.4424901	0.6235849	-1.6633705	C	2.5182748	-0.1065543	3.5133951
O	0.5552090	-0.9352407	-4.7558388	C	1.6383264	2.0676628	2.9183711
O	1.9144616	-0.7539230	-0.3796033	H	0.0461868	2.0766654	1.4523033
H	-1.6293380	0.8197675	0.5457727	C	2.5342069	1.2848162	3.6584507
H	2.1110097	-1.2285850	-2.8109672	H	3.2116853	-0.7257265	4.0858602
H	-1.6068086	0.0146171	-3.9178784	H	1.6449172	3.1541758	3.0262645
H	0.3055325	1.5427419	-0.6423649	H	3.2397224	1.7575300	4.3442907
C	0.2426672	1.8272458	0.8086699	H	-0.0882969	-1.7066501	1.0315430
C	-0.4964403	2.9893909	1.1518221	H	1.5960730	-1.7960544	2.5281847
N	-1.1351469	3.9488648	1.3702456	H	-1.9448026	0.7250350	1.1732060
C	1.5577125	1.7805532	1.3486639	H	-0.6432661	1.9428360	-2.9061203
N	2.6480156	1.7848838	1.7770697	H	1.3632763	-1.5803054	-3.2473097

B + 5a

N _O [⊖] +E				TS _O				N _O -E [⊖]			
C	-1.9747224	1.2096076	-1.1904149	C	-3.6525603	-0.8542870	-0.8006196	C	-3.5929396	-0.8424046	-0.7737612
N	-2.4321518	-0.0856761	-1.0550415	N	-2.3074009	-0.9293912	-1.1196585	N	-2.2451477	-0.8938718	-1.0981472
C	-2.2520081	-0.9340433	0.0705560	C	-1.3004063	-0.1573079	-0.5395514	C	-1.2744904	-0.0875442	-0.5325997
C	-1.5455157	-0.3529498	1.1533143	C	-1.6525775	0.7633192	0.4370990	C	-1.6186176	0.8392211	0.4247692
C	-1.0982046	0.9920960	1.1418711	C	-3.0126262	0.9180115	0.8412408	C	-2.9869743	0.9728124	0.8348526
N	-1.3049092	1.6866370	-0.0835459	N	-3.9406091	0.0778391	0.1737609	N	-3.8945124	0.1005237	0.1881867
O	-2.1501276	1.8817527	-2.2181168	O	-4.5079931	-1.5615832	-1.3464542	O	-4.4319949	-1.5757605	-1.3034953
O	-2.7011527	-2.1028249	0.0022169	O	-0.1153568	-0.4181116	-1.0215552	O	-0.0720304	-0.3454762	-1.0416661
O	-0.5200375	1.6013336	2.0694396	O	-3.4416565	1.7054089	1.7095259	O	-3.4189320	1.7674089	1.6887781
H	-1.3754966	-0.9490306	2.0458670	H	-0.9027600	1.3592909	0.9447630	H	-0.8781099	1.4605040	0.9153944
H	-0.9786662	2.6505812	-0.1294232	H	-4.9204638	0.1666100	0.4415305	H	-4.8755381	0.1717487	0.4584309
H	-2.9052738	-0.4867653	-1.8632523	H	-2.0428465	-1.5968062	-1.8428525	H	-1.9677201	-1.5625549	-1.8157429
C	0.8849054	-1.0750878	-0.2465854	C	1.2892955	0.5948303	-0.5307445	C	1.1338270	0.5083182	-0.5785168
C	0.7309952	-0.6191013	-1.5455369	C	2.2786832	0.3716538	-1.5415184	C	2.2255569	0.2956292	-1.5543655
C	0.0061424	-1.4091371	-2.4842142	C	2.2098432	1.0926972	-2.7505569	C	2.2750749	1.0835674	-2.7099557
N	-0.5723313	-2.0544877	-3.2682524	N	2.1470428	1.7081503	-3.7490652	N	2.3071640	1.7677986	-3.6695337
C	1.2477576	0.5948709	-2.0746935	C	3.2708601	-0.6223333	-1.4346391	C	3.1386241	-0.7560466	-1.4167603
N	1.6555967	1.5782245	-2.5575781	N	4.1142776	-1.4357103	-1.3568797	N	3.9154647	-1.6336505	-1.2968176
C	1.6664871	-0.5365912	0.8456539	C	1.5661214	0.1792985	0.8724945	C	1.4751910	0.1429906	0.8465595
C	2.2414214	0.7542419	0.8638926	C	1.7207404	-1.1708956	1.2253298	C	1.4478373	-1.1889371	1.2828162

C	1.8571085	-1.3757828	1.9707806	C	1.6833021	1.1686857	1.8625795	C	1.8518832	1.1552870	1.7409770
C	3.0071081	1.1703985	1.9509826	C	2.0015585	-1.5233548	2.5474367	C	1.7987409	-1.5044455	2.5989505
H	2.0784765	1.4433913	0.0383061	H	1.5974160	-1.9426180	0.4655206	H	1.1418942	-1.9759410	0.5926220
C	2.6231544	-0.9556900	3.0534750	C	1.9728255	0.8145640	3.1835937	C	2.2062813	0.8390328	3.0558732
H	1.3989010	-2.3668593	1.9787995	H	1.5504440	2.2195106	1.5956159	H	1.8649468	2.1952391	1.4063720
C	3.2053840	0.3199393	3.0449759	C	2.1325560	-0.5324505	3.5290011	C	2.1802649	-0.4927755	3.4882471
H	3.4428207	2.1705191	1.9504679	H	2.1137284	-2.5756368	2.8143225	H	1.7723088	-2.5437550	2.9314347
H	2.7663154	-1.6185144	3.9081317	H	2.0644810	1.5912183	3.9447290	H	2.4948430	1.6341154	3.7456664
H	3.8056575	0.6520760	3.8936800	H	2.3498080	-0.8105848	4.5617415	H	2.4505555	-0.7400286	4.5163636
H	0.4360268	-2.0518744	-0.0560018	H	0.8005688	1.5697580	-0.6166726	H	0.7781786	1.5462123	-0.6408546

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N [⊖] +E				TS _c				N-E [⊖]			
C	0.3638046	-2.0152835	2.2229372	C	-0.7641241	-0.9331991	2.9783995	C	-1.1051217	-0.8505105	3.0020720
H	0.0326770	-1.2375963	2.9219845	H	-1.1190358	0.0845146	3.1844135	H	-1.4365469	0.1827072	3.1648131
H	-0.0304681	-2.9841054	2.5593221	H	-1.4424024	-1.6516844	3.4550293	H	-1.8638366	-1.5395666	3.3903602
H	1.4559236	-2.0483234	2.1877805	H	0.2507749	-1.0640360	3.3626739	H	-0.1488377	-1.0226679	3.5019013
C	-3.3460578	-0.7992633	-0.6559548	C	-3.1880007	-0.9863281	-1.2320259	C	-3.1310026	-1.0870044	-1.4151765
H	-3.9411219	-1.7062102	-0.4812118	H	-3.9382709	-1.6920311	-0.8549303	H	-3.9096681	-1.7452184	-1.0137187
H	-3.6318030	-0.0360813	0.0771941	H	-3.5381937	0.0398974	-1.0657773	H	-3.4808120	-0.0475207	-1.3900456
H	-3.5177416	-0.4272992	-1.6694263	H	-3.0145585	-1.1551909	-2.2977286	H	-2.8847058	-1.3756465	-2.4397377
C	-1.4649901	-1.4451041	0.7315614	C	-1.9184839	-0.9768475	0.8404090	C	-2.0299637	-0.9077216	0.7513724
N	-0.1076214	-1.6995539	0.8730916	N	-0.7197736	-1.1549833	1.5292209	N	-0.9038119	-1.0781541	1.5637711
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C	-1.0799257	-1.0194858	-1.6860954	C	-0.7588481	-1.5289351	-1.2740554	C	-0.7021895	-1.5489865	-1.2233138
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O	-2.2423383	-1.5259145	1.6954949	O	-2.9554979	-0.6637172	1.4317626	O	-3.1069192	-0.5554049	1.2251439
O	2.0131825	-2.0142149	-0.0034027	O	1.5242874	-1.7048787	1.5803380	O	1.3153387	-1.6142970	1.8338772
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C	2.4194164	0.9001478	-0.1724383	C	2.5560548	0.4720850	-0.4004819	C	2.5708272	0.2968470	-0.3374352
C	3.5319953	0.5674419	-0.9946066	C	3.6071449	-0.2626973	-0.9847830	C	3.5847510	-0.5114389	-0.8535995
N	4.4470040	0.3131992	-1.6765575	N	4.4648923	-0.8863458	-1.4904539	N	4.4105277	-1.2159100	-1.3195311
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N	2.9101783	0.7734913	2.3666648	N	3.1918050	1.7896163	1.7269737	N	3.2122356	1.8926591	1.5780704
C	-0.0439570	1.6335938	-0.1865801	C	0.1314921	1.2820367	-0.6545553	C	0.1768472	1.2024449	-0.6433457
C	-0.3648158	1.5106261	1.1847686	C	-0.1424309	1.7287959	0.6532599	C	-0.0969516	1.7237815	0.6332480
C	-1.0275987	2.1531841	-1.0627491	C	-0.7566429	1.6453924	-1.6871568	C	-0.5880201	1.6587553	-1.7302660
C	-1.6124411	1.9098241	1.6577641	C	-1.2661149	2.5140471	0.9159975	C	-1.1103794	2.6686354	0.8165059
H	0.3512528	1.0819621	1.8822107	H	0.5070897	1.4388055	1.4774399	H	0.4744989	1.3846411	1.4966761
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H	-0.8069905	2.2216217	-2.1290266	H	-0.5701376	1.2868192	-2.7011496	H	-0.3958607	1.2537033	-2.7263023
C	-2.5665527	2.4418073	0.7804092	C	-2.1385701	2.8693185	-0.1194081	C	-1.8704164	3.1085132	-0.2730177
H	-1.8490621	1.7924286	2.7157619	H	-1.4684702	2.8389717	1.9377296	H	-1.3114676	3.0558045	1.8168283

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TS _{PT}				⊖ _{N-E}			
C	-0.5069369	0.6241246	0.9172395	C	1.6094814	-1.8944909	-3.5165784
C	-0.5990523	-0.5423626	1.8716338	H	0.9742545	-2.2361091	-4.3443187
C	-0.3399894	-0.3810359	3.2408147	H	2.5032026	-1.4121054	-3.9335143
C	-0.5066813	-1.4494015	4.1296765	H	1.8984987	-2.7436918	-2.8918442
C	-0.9382884	-2.6950963	3.6605594	C	-0.7426606	2.3243331	-3.1517048
C	-1.2055405	-2.8624147	2.2957685	H	0.1061938	2.8932591	-3.5532775
C	-1.0359447	-1.7942417	1.4105794	H	-1.4183518	2.0680370	-3.9779929
H	-0.0051846	0.5860280	3.6205082	H	-1.2731286	2.9209968	-2.4051528
H	-0.2966015	-1.3062517	5.1913786	C	0.4252281	0.2053156	-3.2792802
H	-1.0654659	-3.5296951	4.3523404	N	0.8741015	-0.9527234	-2.6665089
H	-1.5424545	-3.8297316	1.9179959	C	0.6611162	-1.2629576	-1.2885076
H	-1.2398936	-1.9351239	0.3470504	C	-0.0487301	-0.2925228	-0.5280981
C	-0.1644269	0.3617335	-0.5621579	C	-0.5265853	0.9118305	-1.0972480
C	-1.2103223	0.6041103	-1.5450301	N	-0.2694123	1.1053068	-2.4879791
N	-0.8891833	0.2676226	-2.8773324	O	0.6360408	0.4275970	-4.4849048
C	0.2407629	-0.4588613	-3.2476541	O	1.1088788	-2.3471791	-0.8385928
N	1.1106219	-0.8555594	-2.2365370	O	-1.1673259	1.8081632	-0.4786978
C	0.9346732	-0.5421543	-0.8691057	C	-0.2701009	-0.6149680	0.9320124
O	-2.3065876	1.1267990	-1.2783382	C	-1.7675283	-0.3346098	1.3517971
C	-1.8159867	0.6228260	-3.9612992	C	-2.6904480	-1.1047138	0.5173822
O	0.4532876	-0.7541486	-4.4292780	N	-3.4050770	-1.7199085	-0.1636752
C	2.2668941	-1.6613834	-2.6518314	C	-2.0013678	-0.6095459	2.7679903
O	1.7220681	-0.9718594	-0.0152043	N	-2.1565946	-0.8251700	3.9006788
H	1.9289333	-2.5952433	-3.1180108	C	0.6967913	0.0751656	1.8843289
H	2.8744790	-1.1001872	-3.3723045	C	1.6431678	-0.7008724	2.5716450
H	2.8536418	-1.8820954	-1.7565316	C	0.6841488	1.4662548	2.0883493
H	-1.2762704	1.1707077	-4.7424995	C	2.5656133	-0.1039478	3.4385805
H	-2.2580788	-0.2820064	-4.3980725	C	1.6009660	2.0624710	2.9593550
H	-2.6028332	1.2491535	-3.5338244	H	-0.0383675	2.0783140	1.5468749
H	-1.4903210	1.1194995	0.8943955	C	2.5455565	1.2808899	3.6373635
H	0.5528374	1.5461678	-0.2475166	H	3.2967360	-0.7227308	3.9626097
C	0.5220841	1.7748180	1.2143895	H	1.5790145	3.1438986	3.1088853
C	-0.0133314	3.0319743	1.5976985	H	3.2605971	1.7490282	4.3164790
N	-0.4822733	4.0779975	1.8484544	H	-0.1117728	-1.6969813	1.0371049
C	1.8015565	1.4871997	1.7643457	H	1.6591690	-1.7824060	2.4200259
N	2.8705498	1.2985958	2.2055906	H	-1.9602606	0.7376168	1.1466519

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N _O [⊖] +E		TS _O		N _O -E [⊖]			
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N	-0.4889489	-1.2308831	-0.9234193	N	-1.9187506	-0.7259983	-1.1089833

C	-0.4013236	-0.1513068	-1.8586869	C	-0.6588727	0.1700238	-1.0052111	C	-0.9489697	0.0379501	-0.4805170
C	-1.5566523	0.6419544	-1.9863269	C	-1.2277779	1.3500684	-0.5758534	C	-1.2781446	0.8935146	0.5439161
C	-2.7136031	0.4753887	-1.1958141	C	-2.6008698	1.4391076	-0.2083304	C	-2.6295387	1.0249108	0.9858417
N	-2.6759216	-0.6116356	-0.2659274	N	-3.3448068	0.2304707	-0.3489708	N	-3.5786784	0.2182095	0.2949644
O	-1.6152742	-2.4064626	0.6926822	O	-3.4985455	-1.9897159	-0.9214495	O	-4.1359129	-1.3363373	-1.2954136
O	0.6851275	0.0288109	-2.4708685	O	0.6109715	0.0115565	-1.3302006	O	0.2608557	-0.1706473	-1.0000988
O	-3.7379758	1.2039950	-1.2365397	O	-3.1665804	2.4735179	0.2014939	O	-3.0022188	1.7759723	1.9078342
H	-1.5234369	1.4864332	-2.6709163	H	-0.6234762	2.2480386	-0.4936434	H	-0.5237494	1.4684743	1.0689103
C	0.6531729	-2.1246416	-0.7339009	C	3.0665994	0.3143402	-0.7816231	C	-1.5268199	-1.6332583	-2.2004363
H	1.4555490	-1.7691545	-1.3857516	C	3.6672219	1.0487802	-1.8194515	H	-1.0773078	-1.0594611	-3.0191432
H	0.9815932	-2.1018428	0.3137291	N	4.1631389	1.6806043	-2.6787081	H	-0.8008320	-2.3672517	-1.8314890
H	0.3830446	-3.1573249	-0.9915694	C	3.7035797	-0.8687064	-0.3702710	H	-2.4287737	-2.1409205	-2.5487140
C	-3.8154183	-0.8509253	0.6202017	N	4.2559105	-1.8477600	-0.0258095	C	-4.9951804	0.2836701	0.6770142
H	-4.5514325	-0.0664805	0.4238787	C	1.3514860	0.3002966	1.0861353	H	-5.0838872	1.0107481	1.4881996
H	-4.2562789	-1.8379448	0.4254914	C	1.1555421	-1.0530744	1.4085833	H	-5.6009732	0.5996955	-0.1813009
H	-3.4917809	-0.8098320	1.6682884	C	1.1211174	1.2791523	2.0651383	H	-5.3397053	-0.7017542	1.0146842
C	1.9601231	1.0547392	0.0239493	C	1.7730411	0.7256764	-0.2823351	C	1.4574527	0.6168386	-0.4512674
C	3.1149761	0.3001625	0.0847941	C	0.7536244	-1.4194715	2.6946858	C	2.5578266	0.4917688	-1.4375507
C	4.0964665	0.4572261	-0.9368234	H	1.2964065	-1.8158946	0.6429596	C	2.6244003	1.3917309	-2.5060276
N	4.9010968	0.5793177	-1.7751027	C	0.7297056	0.9109371	3.3557533	N	2.6708599	2.1704889	-3.3905522
C	3.4360371	-0.6727920	1.0709345	H	1.2477997	2.3339802	1.8129477	C	3.4435409	-0.5903788	-1.4108634
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C	0.8040751	1.0859021	0.8831613	H	0.5977083	-2.4730302	2.9331104	C	1.7935890	0.1084760	0.9319232
C	0.6014366	0.2435210	2.0056601	H	0.5549798	1.6807771	4.1093452	C	1.7319339	-1.2580426	1.2374608
C	-0.2147677	2.0126529	0.5422745	H	0.2285936	-0.7274673	4.6776329	C	2.2017159	1.0186849	1.9172993
C	-0.5696238	0.3318255	2.7478793	H	1.5858813	1.7867826	-0.4689674	C	2.0803167	-1.7093760	2.5141713
H	1.3525235	-0.4888967	2.2932066	C	-4.7736200	0.2154628	-0.0146207	H	1.4022179	-1.9650993	0.4753413
C	-1.3794364	2.1061021	1.3017023	H	-4.9664606	-0.5138299	0.7822193	C	2.5529872	0.5671331	3.1930013
H	-0.0764960	2.6597673	-0.3240028	H	-5.0431613	1.2199042	0.3220091	H	2.2420972	2.0854055	1.6844954
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H	-0.7189936	-0.3312178	3.6005019	C	-0.8875580	-2.2611215	-1.5479984	H	2.0275470	-2.7750604	2.7444135
H	-2.1582090	2.8128454	1.0151383	H	0.1876354	-2.1330019	-1.6865760	H	2.8659632	1.2835770	3.9546306
H	-2.4788640	1.3243844	2.9888203	H	-1.0821626	-3.0251843	-0.7860005	H	2.7615263	-1.1521722	4.4919236
H	1.9175252	1.7396615	-0.8245533	H	-1.3520804	-2.5709449	-2.4925146	H	1.1206688	1.6623810	-0.4092388

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N [⊕] +E				TS _c				N-E [⊖]			
C	-1.5277328	0.7575121	1.2681975	C	-1.8113810	0.9045953	0.8812911	C	-2.2141186	0.1382257	0.5076907
N	-1.3171869	-0.5805624	1.5679147	N	-1.4547940	-0.2549504	1.5678130	N	-1.6090244	-0.8119615	1.3370486
C	-1.5356928	-1.6474813	0.6396189	C	-1.2976622	-1.5151170	0.9524812	C	-0.8237318	-1.8700589	0.8701384
C	-1.8610986	-1.2530448	-0.6751799	C	-1.3342013	-1.5115633	-0.4941662	C	-0.4724232	-1.8339846	-0.5807446
C	-2.0292060	0.0928752	-1.0738559	C	-1.9090246	-0.3960781	-1.2199936	C	-1.4053787	-1.0795463	-1.4761082
N	-1.8445022	1.0688195	-0.0477975	N	-2.0574245	0.7963440	-0.4889050	N	-2.1433657	-0.0623414	-0.8767610
O	-1.4283707	1.6390110	2.1376117	O	-1.9264504	1.9850100	1.4655702	O	-2.8299715	1.0913264	0.9775275
O	-1.3833674	-2.8321460	1.0260932	O	-1.0431691	-2.5270003	1.6236790	O	-0.3783712	-2.7321082	1.6268251
O	-2.3111683	0.4764422	-2.2358454	O	-2.1716134	-0.4374921	-2.4349901	O	-1.4280779	-1.2725889	-2.6939583
H	-2.0151212	-2.0312776	-1.4185347	H	-1.5220719	-2.4857009	-0.9442641	H	-0.3838829	-2.8626898	-0.9485840

C	-2.0410548	2.4856507	-0.3578654	C	-2.4404315	2.0350153	-1.1759138	C	-2.8520368	0.9212180	-1.7091972
H	-3.0023976	2.8436762	0.0381902	H	-3.3691516	2.4339094	-0.7504497	H	-3.9141599	0.9465518	-1.4411904
H	-1.2332503	3.0740635	0.0904878	H	-1.6403975	2.7774461	-1.0622449	H	-2.4098435	1.9128511	-1.5507244
H	-2.0276226	2.5897304	-1.4459350	H	-2.5817452	1.7958039	-2.2328363	H	-2.7331236	0.6196269	-2.7525553
C	-0.9230491	-0.8891799	2.9436520	C	-1.2188199	-0.1106918	3.0082460	C	-1.7915975	-0.6163390	2.7823067
H	-0.0474520	-0.2897841	3.2215520	H	-0.4440845	0.6474836	3.1780444	H	-1.3693229	0.3533553	3.0743137
H	-1.7397498	-0.6685328	3.6449995	H	-2.1396194	0.1974329	3.5190113	H	-2.8580223	-0.6377424	3.0345880
H	-0.6755234	-1.9532388	2.9806383	H	-0.8874288	-1.0813533	3.3862933	H	-1.2670462	-1.4260693	3.2953196
C	1.0229565	-1.4200626	-1.0636178	C	0.6406503	-1.4002356	-0.9933255	C	1.0176868	-1.1656687	-0.7942132
C	1.2842562	-2.5510381	-0.3036106	C	1.2993229	-2.5723834	-0.4689929	C	2.1063561	-2.0066731	-0.1768418
C	0.9860932	-3.8299613	-0.8491526	C	1.0340424	-3.8131485	-1.0779222	C	2.3658830	-3.2499363	-0.7551891
N	0.7558867	-4.8799765	-1.3097713	N	0.7924487	-4.8356389	-1.6058117	N	2.5511269	-4.2925646	-1.2787116
C	1.7936648	-2.5688847	1.0209633	C	2.1234344	-2.6078561	0.6691119	C	2.8008487	-1.6831599	0.9868490
N	2.2363120	-2.6202273	2.1026396	N	2.8486731	-2.6671858	1.5929292	N	3.4196254	-1.4153419	1.9568089
C	1.2270441	-0.0268432	-0.7711487	C	1.0375319	-0.0215788	-0.6398924	C	0.9831146	0.3013799	-0.4291953
C	1.5714497	0.4952128	0.5025645	C	1.3949456	0.3783046	0.6664371	C	0.9644818	0.7603878	0.9025942
C	1.0025158	0.8969236	-1.8198360	C	0.9430200	0.9775846	-1.6250092	C	0.8277760	1.2517132	-1.4476207
C	1.6863224	1.8578177	0.7063734	C	1.6472765	1.7099008	0.9671104	C	0.7916302	2.1080439	1.1990726
H	1.7278700	-0.1704131	1.3483463	H	1.4476275	-0.3556066	1.4687993	H	1.0723055	0.0559895	1.7267513
C	1.1263162	2.2675144	-1.6309714	C	1.1976044	2.3206319	-1.3411567	C	0.6504218	2.6117346	-1.1708594
H	0.7073184	0.5242218	-2.8017052	H	0.6451201	0.7012751	-2.6383283	H	0.8237199	0.9239938	-2.4895996
C	1.4576465	2.7581189	-0.3550444	C	1.5423648	2.6948127	-0.0322637	C	0.6229566	3.0440683	0.1636034
H	1.9241605	2.2574551	1.6920859	H	1.9071345	2.0131547	1.9819890	H	0.7696631	2.4535700	2.2335070
H	0.9351107	2.9417812	-2.4632797	H	1.1103217	3.0587167	-2.1365049	H	0.5271464	3.3113979	-1.9958084
H	0.6633140	-1.6288647	-2.0727953	H	0.3856952	-1.5020097	-2.0521535	H	1.1178048	-1.2348577	-1.8877615
O	1.5601758	4.0770294	-0.0401879	O	1.7904991	3.9783636	0.3675933	O	0.4401195	4.3441094	0.5570681
C	1.2885526	5.0480256	-1.0756484	C	1.6511282	5.0271093	-0.6123122	C	0.2375383	5.3329849	-0.4714447
H	0.2580942	4.9455963	-1.4486471	H	0.6237990	5.0663914	-1.0073133	H	-0.6641570	5.1115864	-1.0642213
H	1.4129195	6.0245857	-0.5978743	H	1.8756091	5.9570799	-0.0801192	H	0.1047054	6.2829576	0.0565365
H	2.0014461	4.9471221	-1.9076920	H	2.3639046	4.8946989	-1.4411556	H	1.1121504	5.4007653	-1.1375158

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TS _{PT}				Θ _{N-E}			
C	0.9883407	0.1737075	-0.5803787	C	1.5653172	-1.9453348	-3.6030897
C	0.3189307	1.4990853	-0.3007915	H	0.9077879	-2.2945473	-4.4100365
C	0.3699938	2.1699225	0.9347012	H	2.4388591	-1.4516786	-4.0485923
C	-0.2871529	3.3833214	1.1215988	H	1.8848818	-2.7912067	-2.9888058
C	-1.0319814	3.9576384	0.0763692	C	-0.8213805	2.2455155	-3.1564201
C	-1.1006698	3.3032256	-1.1629395	H	0.0079765	2.8237601	-3.5845631
C	-0.4209031	2.0914577	-1.3356731	H	-1.5208711	1.9831995	-3.9607434
H	0.9159460	1.7300531	1.7657165	H	-1.3334946	2.8355653	-2.3920481
H	-0.2398417	3.9008457	2.0813610	C	0.3657200	0.1404154	-3.3250015
H	-1.6631675	3.7233174	-1.9954175	N	0.8465938	-1.0130599	-2.7287393
H	-0.4746405	1.5943723	-2.3074281	C	0.6780176	-1.3286997	-1.3456307
O	-1.6468181	5.1513314	0.3635188	C	-0.0151465	-0.3664918	-0.5595884
C	-2.4220506	5.7724730	-0.6797142	C	-0.5245182	0.8322107	-1.1125163
H	-3.2557991	5.1256644	-0.9962390	N	-0.3140910	1.0306470	-2.5104094

H	-2.8197772	6.6939782	-0.2417124	O	0.5363082	0.3673124	-4.5362661
H	-1.7941221	6.0199957	-1.5503728	O	1.1474099	-2.4113126	-0.9138521
H	1.1195560	0.1072435	-1.6692970	O	-1.1548256	1.7224224	-0.4732332
C	-1.4519798	-3.3603612	0.2666438	C	-0.1960755	-0.7033003	0.9032620
N	-1.0795759	-2.4920020	1.2871737	C	-1.6878158	-0.4288352	1.3594923
C	-0.2908897	-1.3325040	1.0968485	C	-2.6321728	-1.1817666	0.5335508
C	0.2603288	-1.1493296	-0.2362122	N	-3.3621164	-1.7846159	-0.1425286
C	-0.2897023	-1.8985493	-1.3598381	C	-1.8917949	-0.7267010	2.7751098
N	-1.0404346	-3.0461403	-1.0265746	N	-2.0255198	-0.9620641	3.9067059
O	-2.1363243	-4.3647997	0.4950536	C	0.7788372	-0.0289971	1.8550884
O	-0.0465913	-0.5772731	2.0487859	C	1.6092613	-0.8139498	2.6632672
O	-0.0850821	-1.6126139	-2.5524307	C	0.8807701	1.3718837	1.9613235
C	-1.4967156	-3.9517301	-2.0904581	C	2.5286047	-0.2411781	3.5521298
H	-1.1928540	-4.9785640	-1.8558056	C	1.7831179	1.9585510	2.8432328
H	-2.5899422	-3.9135446	-2.1821621	H	0.2439732	2.0012444	1.3379537
H	-1.0360358	-3.6243090	-3.0256821	C	2.6151025	1.1555857	3.6455837
C	-1.5660314	-2.8241873	2.6331573	H	3.1596814	-0.8890384	4.1587185
H	-2.6630619	-2.8211641	2.6508202	H	1.8606599	3.0441853	2.9250037
H	-1.2056438	-3.8179736	2.9259053	H	-0.0371585	-1.7868729	0.9916627
H	-1.1799328	-2.0666522	3.3198761	H	1.5461241	-1.9026047	2.6004667
H	1.6332943	-1.4342739	-0.0122856	H	-1.8781065	0.6477801	1.1757311
C	2.4133488	-0.1765409	-0.0166276	C	4.3378652	1.0481213	5.3244492
C	2.8143149	0.0990735	1.3191927	H	3.7576439	0.4146553	6.0141781
N	3.2033766	0.2802234	2.4102880	H	5.0164616	0.4194172	4.7262095
C	3.4782324	-0.1222411	-0.9547309	H	4.9227562	1.7743047	5.8986654
N	4.3264621	-0.1349308	-1.7657447	O	3.4712278	1.8301920	4.4803975

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N _O [⊖] +E				TS _O			N _O -E [⊖]				
C	-1.0342405	-1.3460513	-1.2926806	C	-2.4550586	-1.1101567	-1.4630676	C	-3.6805146	-0.7108586	0.4138716
N	0.1342247	-0.7000870	-1.6615607	N	-1.0637670	-1.1376382	-1.5664761	N	-2.6069493	-0.7901618	-0.4814165
C	0.2082799	0.6951640	-1.9755138	C	-0.3026290	0.0300439	-1.6171109	C	-1.5006069	0.0373197	-0.3703284
C	-1.0142646	1.3944174	-1.9382570	C	-0.9320728	1.2543738	-1.5766620	C	-1.4166952	0.9701494	0.6365458
C	-2.2327925	0.8186669	-1.5260372	C	-2.3460614	1.3754531	-1.4456384	C	-2.4666749	1.1169124	1.5923510
N	-2.1907929	-0.5825852	-1.2385537	N	-3.0551495	0.1399062	-1.3938762	N	-3.5771220	0.2414705	1.4188635
O	-1.0457232	-2.5588533	-1.0179721	O	-3.1142770	-2.1572503	-1.4229716	O	-4.6694124	-1.4468218	0.3176386
O	1.3346897	1.1959930	-2.2299406	O	1.0078935	-0.1395791	-1.6831298	O	-0.6082504	-0.1954037	-1.3312344
O	-3.3216919	1.4331236	-1.3737912	O	-2.9691178	2.4546987	-1.3829235	O	-2.4590041	1.9359467	2.5319257
H	-0.9937876	2.4660065	-2.1228091	H	-0.3451458	2.1668997	-1.6206137	H	-0.5405225	1.5966594	0.7578679
C	3.4066987	0.1936568	0.6640541	C	3.2922325	0.2759715	-0.6972158	C	1.2681242	0.4539531	-2.7323849
C	4.5678530	0.7605702	0.0675849	C	4.0661701	0.9151142	-1.6806135	C	0.8195192	1.2495735	-3.7915104
N	5.5219680	1.2226326	-0.4260143	N	4.7044590	1.4702007	-2.4988080	N	0.4375345	1.9430824	-4.6658425
C	3.5716976	-1.1296620	1.1516458	C	3.8645128	-0.8240357	-0.0395769	C	2.1472319	-0.5984407	-3.0065699
N	3.7422425	-2.2193728	1.5409062	N	4.3644824	-1.7331769	0.5150094	N	2.8988599	-1.4768017	-3.2364072
C	0.9342204	0.6239510	1.1977101	C	1.2156467	0.4039125	0.7753207	C	1.5727483	0.2459414	-0.2342167
C	0.5350815	-0.6304706	1.7407042	C	1.0495286	-0.9081547	1.2606633	C	1.7366681	-1.1007642	0.1298177
C	-0.0569653	1.6332288	1.0793589	C	0.6333647	1.4571145	1.4925249	C	2.2719312	1.2250736	0.4781998

C	2.2369244	0.9386411	0.7018272	C	1.9138462	0.6912902	-0.5088630	C	0.6821563	0.6458816	-1.3834974
C	-0.7730537	-0.8557342	2.1150085	C	0.3457094	-1.1507341	2.4330947	C	2.5820731	-1.4564588	1.1758078
H	1.2522850	-1.4409672	1.8508178	H	1.4534159	-1.7502940	0.6998711	H	1.1866618	-1.8749699	-0.4062218
C	-1.3693385	1.4259840	1.4778428	C	-0.0657610	1.2328263	2.6826925	C	3.1315954	0.8851219	1.5287601
H	0.2217872	2.6012471	0.6617586	H	0.7241254	2.4783880	1.1177011	H	2.1479695	2.2783112	0.2155426
C	-1.7446892	0.1627141	1.9648141	C	-0.2141289	-0.0800276	3.1562171	C	3.2884293	-0.4651729	1.8810806
H	-1.0866110	-1.8262008	2.4996634	H	0.2081064	-2.1675576	2.8035436	H	2.7080662	-2.5011922	1.4641498
H	-2.1023284	2.2171103	1.3400360	H	-0.5012976	2.0780570	3.2128198	H	3.6581607	1.6738775	2.0635265
H	2.3295975	1.9333195	0.2614380	H	1.7643496	1.7255872	-0.8326370	H	0.3479533	1.6873199	-1.2738161
C	1.3497773	-1.5134367	-1.6740403	C	-0.4396027	-2.4677804	-1.6006849	C	-2.6612626	-1.7774725	-1.5722313
H	2.1856632	-0.8444112	-1.8947241	H	0.6413584	-2.3336061	-1.6702319	H	-2.6221758	-1.2657084	-2.5408655
H	1.4958331	-1.9872747	-0.6946239	H	-0.6919137	-3.0180348	-0.6859768	H	-1.8123935	-2.4666859	-1.4928686
H	1.2819700	-2.3012245	-2.4363381	H	-0.8064771	-3.0283631	-2.4691179	H	-3.6002198	-2.3265927	-1.4753553
C	-3.4136838	-1.2840229	-0.8428416	C	-4.5173846	0.1481672	-1.2690626	C	-4.7081455	0.3168600	2.3524710
H	-3.3306347	-1.6493341	0.1893346	H	-4.8198981	-0.3718374	-0.3513949	H	-4.8336140	-0.6424643	2.8699373
H	-4.2375159	-0.5687552	-0.9140184	H	-4.8386553	1.1923241	-1.2325644	H	-4.4864469	1.1067914	3.0745637
H	-3.5935553	-2.1371906	-1.5091502	H	-4.9716314	-0.3565419	-2.1311020	H	-5.6303076	0.5521260	1.8066921
O	-3.0101465	-0.1798142	2.3029126	O	-0.8902496	-0.4230578	4.2964359	O	4.0947170	-0.9151165	2.8952694
C	-4.0661830	0.7794028	2.0453016	C	-1.4990790	0.6362461	5.0620944	C	4.8346658	0.0649311	3.6494316
H	-4.9941804	0.2608453	2.3042750	H	-1.9766755	0.1436977	5.9153327	H	5.4039149	-0.5044497	4.3915346
H	-3.9463000	1.6683717	2.6821295	H	-0.7429469	1.3504634	5.4241089	H	5.5288650	0.6245630	3.0027138
H	-4.0713945	1.0658814	0.9818436	H	-2.2600124	1.1679846	4.4695488	H	4.1582846	0.7664085	4.1630205

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N [⊕] +E				TS _c			N-E [⊖]				
C	-0.8244787	0.9310317	1.5956638	C	-1.7296928	0.6843255	1.0551454	C	-2.1379887	0.0358856	0.5016439
N	-0.6230422	-0.3872993	1.9743192	N	-1.1675252	-0.3819793	1.7561186	N	-1.5021163	-0.8350457	1.3929770
C	-1.0225028	-1.5209220	1.1891610	C	-1.0210355	-1.6798698	1.2257752	C	-0.7456984	-1.9420776	0.9985195
C	-1.5451278	-1.2225032	-0.0842707	C	-1.3006347	-1.8109364	-0.1910908	C	-0.4563965	-2.0495822	-0.4613078
C	-1.7063890	0.0912044	-0.5723378	C	-2.1038604	-0.8129780	-0.8760762	C	-1.4218058	-1.3776708	-1.3855305
N	-1.3266550	1.1417363	0.3183528	N	-2.2177305	0.4286184	-0.2286212	N	-2.1284919	-0.3006106	-0.8584417
O	-0.5541157	1.8718693	2.3648318	O	-1.8190391	1.8061071	1.5588134	O	-2.7301644	1.0340130	0.9019454
O	-0.8599472	-2.6723144	1.6653368	O	-0.5804766	-2.6084372	1.9202602	O	-0.2737669	-2.7311972	1.8173734
O	-2.1549115	0.4086077	-1.7038090	O	-2.5852529	-0.9905287	-2.0089686	O	-1.4980207	-1.6882764	-2.5773976
H	-1.8307171	-2.0507085	-0.7283972	H	-1.4996171	-2.8331977	-0.5125023	H	-0.3839151	-3.1089334	-0.7330657
C	-1.5309854	2.5206936	-0.1261336	C	-2.8203246	1.5693475	-0.9271019	C	-2.8614468	0.6080021	-1.7519857
H	-2.5904212	2.8059875	-0.0478864	H	-3.6804838	1.9490800	-0.3626603	H	-3.9111875	0.6742533	-1.4447151
H	-0.9281242	3.1797069	0.5041584	H	-2.0723626	2.3657086	-1.0321977	H	-2.4008570	1.6031057	-1.7066829
H	-1.2183346	2.6021614	-1.1718468	H	-3.1391794	1.2219841	-1.9129977	H	-2.7893321	0.2063193	-2.7655033
C	-0.0134377	-0.6064564	3.2865358	C	-0.6832605	-0.0846671	3.1079623	C	-1.6099486	-0.4888882	2.8168144
H	0.8691376	0.0355823	3.3914850	H	0.0445608	0.7351401	3.0604838	H	-1.1825708	0.5087121	2.9785925
H	-0.7189957	-0.3719891	4.0965956	H	-1.5158920	0.2115820	3.7581543	H	-2.6610277	-0.4876986	3.1282356
H	0.2757729	-1.6596134	3.3401736	H	-0.2095755	-0.9905782	3.4950896	H	-1.0506327	-1.2372101	3.3836052
C	1.3889855	-1.6629904	-0.9445665	C	0.4974175	-1.6092372	-1.0433342	C	1.0304609	-1.4079374	-0.7959486
C	1.6060459	-2.8103521	-0.1840492	C	1.3294649	-2.7076904	-0.5858814	C	2.1355092	-2.2080969	-0.1529286
C	1.1381721	-4.0579918	-0.6731875	C	1.0339506	-4.0015768	-1.0474571	C	2.3374345	-3.5123294	-0.6058374
N	0.7570745	-5.0862283	-1.0832157	N	0.7604303	-5.0723615	-1.4521763	N	2.4705634	-4.6096013	-1.0233209

C	2.2296239	-2.8622781	1.0879257	C	2.3598922	-2.6097907	0.3620269	C	2.9107474	-1.7758822	0.9206962
N	2.7695242	-2.9427643	2.1235609	N	3.2550428	-2.5571632	1.1243951	N	3.5977619	-1.4209074	1.8139748
C	1.6792920	-0.2950452	-0.6775673	C	0.8664318	-0.1932281	-0.8598431	C	1.0144145	0.0812637	-0.5527695
C	2.1455133	0.2127947	0.5655518	C	1.4227390	0.3261752	0.3270465	C	1.0540863	0.6539393	0.7305352
C	1.3853843	0.6594243	-1.6907890	C	0.5065601	0.7384886	-1.8547760	C	0.7756508	0.9508576	-1.6297997
C	2.2416347	1.5662313	0.8028616	C	1.6024029	1.6896175	0.5175280	C	0.8556750	2.0160636	0.9349085
H	2.4008251	-0.4685199	1.3744156	H	1.6835516	-0.3444235	1.1448978	H	1.2150950	0.0226553	1.6046031
C	1.5047202	2.0168858	-1.4789165	C	0.6849614	2.1058578	-1.6872378	C	0.5723093	2.3168878	-1.4491422
H	1.0254539	0.3064965	-2.6592092	H	0.0459030	0.3786548	-2.7777222	H	0.7135074	0.5422627	-2.6416306
C	1.8730847	2.5185815	-0.1954180	C	1.2288502	2.6283361	-0.4825400	C	0.6026305	2.8931035	-0.1524255
H	2.5593179	1.9023403	1.7869417	H	2.0076792	2.0297576	1.4684030	H	0.8758581	2.3932925	1.9555633
H	1.2380180	2.7001477	-2.2825269	H	0.3731368	2.7727268	-2.4888500	H	0.3722807	2.9320268	-2.3245756
H	0.9224754	-1.8541970	-1.9139716	H	0.0767775	-1.7999392	-2.0359534	H	1.0800343	-1.5717797	-1.8832251
C	1.4706837	4.8212067	-0.9421249	C	0.7710136	4.9172466	-1.2332507	C	-0.1308931	5.0514231	-1.0558122
H	0.4067728	4.7302860	-1.2197111	H	-0.3308086	4.8271871	-1.2529649	H	-1.1370872	4.7178160	-1.3726257
H	1.6454646	5.8303997	-0.5571095	H	1.0314315	5.9398668	-0.9406895	H	-0.1959377	6.0961983	-0.7329662
H	2.0819823	4.6909463	-1.8463353	H	1.1499598	4.7541036	-2.2525597	H	0.5360372	5.0143294	-1.9291622
N	1.8459678	3.8514746	0.0856748	N	1.3853967	3.9852332	-0.2907259	N	0.4018405	4.2500768	0.0434968
C	1.9671774	4.3097601	1.4724684	C	1.6997519	4.4877356	1.0452836	C	0.1539301	4.7396780	1.3980138
H	1.2391354	3.7876609	2.1135484	H	0.9092892	4.2434141	1.7780717	H	-0.7612136	4.3050980	1.8419016
H	2.9811842	4.1388116	1.8662599	H	2.6509353	4.0727250	1.4089704	H	1.0015311	4.5116346	2.0601546
H	1.7634271	5.3841044	1.5074754	H	1.8082251	5.5763599	0.9972638	H	0.0432868	5.8290468	1.3653305

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TS _{PT}	Θ _{N-E}		
C	1.0873234	-0.1543076	-0.5610769
C	0.5139130	1.2309058	-0.3899905
C	0.4984673	1.9485364	0.8167224
C	-0.0653104	3.2205029	0.9064920
C	-0.6522164	3.8510565	-0.2225422
C	-0.6569003	3.1147976	-1.4361230
C	-0.0757683	1.8494927	-1.5067596
H	0.9133349	1.4967045	1.7149702
H	-0.0499904	3.7243321	1.8717721
H	-1.1057663	3.5320192	-2.3361349
H	-0.0917006	1.3200650	-2.4633689
N	-1.1793601	5.1330322	-0.1478264
C	-2.0144642	5.6194804	-1.2434392
H	-2.9301789	5.0134730	-1.3801878
H	-2.3095586	6.6529898	-1.0309933
H	-1.4575732	5.6217979	-2.1915237
C	-1.4042795	5.7306112	1.1663262
H	-2.1330036	5.1599428	1.7727206
H	-0.4644083	5.8008306	1.7325228
H	-1.7858259	6.7486919	1.0309097
H	1.2826347	-0.2867819	-1.6343334
C	-1.6571452	-3.4669132	0.2694612
C	1.6355316	-1.8730882	-3.5861574
H	0.9969960	-2.2377653	-4.4015323
H	2.4983217	-1.3513237	-4.0205026
H	1.9740730	-2.7121708	-2.9726962
C	-0.8798853	2.2412467	-3.1422277
H	-0.0641245	2.8461772	-3.5595642
H	-1.5637835	1.9629733	-3.9546262
H	-1.4164110	2.8116080	-2.3796427
C	0.3717980	0.1742882	-3.3097594
N	0.8805664	-0.9673670	-2.7146032
C	0.7071389	-1.2956113	-1.3343832
C	-0.0211750	-0.3590051	-0.5496116
C	-0.5621256	0.8255875	-1.1025496
N	-0.3428690	1.0385737	-2.4976510
O	0.5482630	0.4132415	-4.5182164
O	1.2040167	-2.3670527	-0.9048714
O	-1.2272033	1.6930216	-0.4667184
C	-0.2062458	-0.7095624	0.9101273
C	-1.7144359	-0.4820236	1.3461305
C	-2.6267152	-1.2559371	0.5039415
N	-3.3277683	-1.8765406	-0.1868464
C	-1.9297125	-0.7928373	2.7568105

N	-1.2888176	-2.5804351	1.2752367	N	-2.0764635	-1.0402225	3.8843365
C	-0.4026625	-1.4912414	1.0919489	C	0.7306070	-0.0161067	1.8832981
C	0.2432638	-1.4064881	-0.2078057	C	1.5324017	-0.7781014	2.7455071
C	-0.2827302	-2.1709234	-1.3324400	C	0.8414415	1.3822629	1.9668710
N	-1.1383601	-3.2447891	-1.0036867	C	2.4117355	-0.1867148	3.6528153
O	-2.4281357	-4.4082654	0.4923577	C	1.7086645	1.9932248	2.8700686
O	-0.1615368	-0.7173774	2.0296680	H	0.2387607	2.0033656	1.3020475
O	0.0233220	-1.9614758	-2.5194588	C	2.5122031	1.2250497	3.7557033
C	-1.5878801	-4.1660537	-2.0568192	H	3.0198938	-0.8324930	4.2841882
H	-1.3755605	-5.1993432	-1.7582672	H	1.7595850	3.0809299	2.8842813
H	-2.6670449	-4.0565315	-2.2255119	H	-0.0185257	-1.7891715	0.9932495
H	-1.0439506	-3.9161500	-2.9710179	H	1.4792861	-1.8689037	2.7012071
C	-1.8842306	-2.8147354	2.5977513	H	-1.9289216	0.5904859	1.1645150
H	-2.9771136	-2.7368114	2.5400789	N	3.3453701	1.8288832	4.6872499
H	-1.6150562	-3.8155729	2.9572495	C	3.6327230	3.2560065	4.5625220
H	-1.4911334	-2.0532559	3.2760876	H	2.7092303	3.8500944	4.6186729
H	1.5737827	-1.7754822	0.1237603	H	4.2733287	3.5615249	5.3971516
C	2.4448931	-0.5790484	0.1133059	H	4.1479310	3.5036882	3.6151761
C	2.7804504	-0.2528350	1.4554463	C	4.3409413	1.0142851	5.3794112
N	3.1110029	-0.0323546	2.5586070	H	3.8606923	0.2014691	5.9431565
C	3.5667286	-0.6554535	-0.7536871	H	5.0791826	0.5672052	4.6868353
N	4.4595425	-0.7750604	-1.5063164	H	4.8757455	1.6446595	6.0983858

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N _O [⊖] +E				TS _O				N _O -E [⊖]			
C	-1.0462467	-1.5167664	1.0502505	C	-3.6409130	-0.8824895	0.9001598	C	-3.6927107	-0.8428404	0.8887947
N	-1.4368755	-1.0794618	-0.2040782	N	-2.7269242	-0.9558669	-0.1534768	N	-2.7593940	-0.9157814	-0.1518887
C	-2.1666135	0.1323438	-0.4353526	C	-1.7230916	-0.0019650	-0.3458814	C	-1.7096738	-0.0155221	-0.2582003
C	-2.4785147	0.8848397	0.7149305	C	-1.6142893	1.0553834	0.5418790	C	-1.5452877	0.9850490	0.6717510
C	-2.0551603	0.5422851	2.0131077	C	-2.4942398	1.1982811	1.6481295	C	-2.4499507	1.1292629	1.7656497
N	-1.3667212	-0.7080733	2.1304023	N	-3.4967988	0.1880559	1.7704987	N	-3.5099918	0.1780017	1.8116712
O	-0.4375536	-2.5908671	1.2051184	O	-4.5345481	-1.7270142	1.0569299	O	-4.6314339	-1.6424508	0.9844274
O	-2.4547824	0.4445630	-1.6198549	O	-0.9824825	-0.2376642	-1.3976377	O	-0.9564750	-0.2537124	-1.3282832
O	-2.2220532	1.2371805	3.0518022	O	-2.4456711	2.1237136	2.4876503	O	-2.3620866	2.0070887	2.6467593
H	-2.9784966	1.8409796	0.5767628	H	-0.8276863	1.7930192	0.4351711	H	-0.7055894	1.6687595	0.6245751
C	-1.0659654	-1.9285118	-1.3355515	C	-2.8282102	-2.0705481	-1.1069700	C	-2.9041484	-1.9745614	-1.1642086
H	-1.3507763	-1.3958233	-2.2467406	H	-3.0436152	-1.6863063	-2.1115367	H	-3.0592041	-1.5273613	-2.1531726
H	0.0163112	-2.1087095	-1.3292376	H	-1.8820165	-2.6238194	-1.1320132	H	-2.0002674	-2.5944868	-1.1854523
H	-1.5844329	-2.8959217	-1.2838903	H	-3.6379984	-2.7237444	-0.7742134	H	-3.7688908	-2.5815192	-0.8877597
C	-0.9822022	-1.2075492	3.4505359	C	-4.4576260	0.2543415	2.8776700	C	-4.4940894	0.2460455	2.8993750
H	-1.3008862	-0.4647597	4.1866332	H	-4.2171342	1.1428397	3.4673573	H	-4.2241483	1.0936683	3.5343982
H	-1.4681737	-2.1718121	3.6507957	H	-5.4805320	0.3271117	2.4868457	H	-5.5005998	0.3888599	2.4867875
H	0.1043353	-1.3444840	3.5063165	H	-4.3783816	-0.6447451	3.5018987	H	-4.4754269	-0.6830054	3.4827826
C	0.5118387	1.0182921	-2.4566584	C	0.4351897	0.7530618	-1.7236195	C	0.2622838	0.6592032	-1.6175917
C	0.7300671	0.2472051	-3.5996273	C	0.7751684	0.4361445	-3.0923916	C	0.6492560	0.4116570	-3.0280710
C	0.0724191	0.6027366	-4.8073760	C	0.0689937	1.0586551	-4.1365249	C	-0.0210720	1.0916268	-4.0500261
N	-0.4710471	0.8938087	-5.8027409	N	-0.5229446	1.5997407	-4.9973694	N	-0.5895893	1.6904292	-4.8926527

C	1.5405419	-0.9128080	-3.6791436	C	1.6983482	-0.5634583	-3.4408791	C	1.5674898	-0.5843276	-3.3747785
N	2.1983720	-1.8766228	-3.7759266	N	2.4811058	-1.3837609	-3.7532911	N	2.3514557	-1.4130642	-3.6717311
C	0.9955278	0.8888990	-1.1300673	C	1.3854850	0.4398628	-0.6307238	C	1.3280271	0.3882252	-0.5912058
C	1.8740124	-0.1293471	-0.6579529	C	1.7958256	-0.8735918	-0.3445189	C	1.6602088	-0.9153875	-0.1974279
C	0.5154794	1.8196966	-0.1625469	C	1.9046132	1.4745866	0.1647490	C	2.0421182	1.4493893	-0.0188333
C	2.2008324	-0.2401338	0.6744076	C	2.6955982	-1.1461069	0.6793692	C	2.6663837	-1.1579793	0.7340517
H	2.2968529	-0.8547772	-1.3505087	H	1.3856932	-1.7020287	-0.9230573	H	1.1166598	-1.7599484	-0.6239323
C	0.8447267	1.7297266	1.1706106	C	2.8186520	1.2250133	1.1838208	C	3.0582073	1.2280326	0.9083778
H	-0.1509965	2.6195532	-0.4887357	H	1.5991232	2.5064563	-0.0265205	H	1.8054755	2.4770762	-0.3067911
C	1.6622783	0.6632275	1.6461241	C	3.2357149	-0.1013259	1.4811325	C	3.3919768	-0.0886875	1.3257062
H	2.8587321	-1.0489430	0.9847366	H	2.9778254	-2.1816657	0.8612411	H	2.8870028	-2.1895091	1.0031540
H	0.4205086	2.4501941	1.8655955	H	3.2014206	2.0670391	1.7576379	H	3.5862772	2.0880999	1.3163233
H	-0.1777453	1.8507329	-2.6133578	H	-0.0184928	1.7451713	-1.6327810	H	-0.1262705	1.6828681	-1.5180857
N	1.9141097	0.5052702	2.9728019	N	4.1103322	-0.3668115	2.5148289	N	4.3667905	-0.3183060	2.2828698
C	2.8328881	-0.5343818	3.4411542	C	4.6722651	-1.7071613	2.6604167	C	4.8513522	-1.6800533	2.4946091
H	2.8788720	-0.4979479	4.5331334	H	5.3106002	-1.7283017	3.5498988	H	5.5862791	-1.6713346	3.3068282
H	2.4865382	-1.5361772	3.1438053	H	3.8783537	-2.4558257	2.8009655	H	4.0309120	-2.3477286	2.7956334
H	3.8482942	-0.3803229	3.0439402	H	5.2796474	-2.0046512	1.7861548	H	5.3305011	-2.1035865	1.5920746
C	1.3140783	1.4130665	3.9534165	C	4.7938773	0.7373418	3.1831534	C	5.2555197	0.7740596	2.6712458
H	1.7462840	2.4245557	3.8840903	H	5.4443959	1.3064426	2.4939809	H	5.8636109	1.1454313	1.8251324
H	0.2246322	1.4764660	3.8058534	H	4.0717751	1.4353263	3.6325999	H	4.6847739	1.6189444	3.0835059
H	1.5036254	1.0213281	4.9570774	H	5.4132034	0.3333417	3.9908165	H	5.9320194	0.4175018	3.4555377

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N [⊖] +E				TS _C				N-E [⊖]			
C	0.9573731	-5.1524159	1.4732626	C	0.6518995	-5.3221264	-1.4110990	C	0.7366859	-5.0405513	-1.6094132
C	0.1785518	-3.9914385	1.6017404	C	-0.1211886	-4.7054153	-0.4126811	C	0.6274325	-4.7493553	-0.2430009
C	0.4503145	-2.8822170	0.7913467	C	0.1119199	-3.3690854	-0.0792444	C	0.9567661	-3.4680458	0.2239194
C	1.4859848	-2.8964139	-0.1524049	C	1.1087634	-2.6125561	-0.7215656	C	1.3956977	-2.4631680	-0.6442471
C	2.2497910	-4.0710343	-0.2686664	C	1.8984043	-3.2651219	-1.6944057	C	1.5009278	-2.7769861	-2.0136440
C	1.9991186	-5.1859628	0.5311941	C	1.6716333	-4.5911305	-2.0462119	C	1.1787666	-4.0412226	-2.4959311
H	-0.6374827	-3.9382492	2.3215269	H	-0.8966679	-5.2554462	0.1182164	H	0.2889589	-5.5009474	0.4687634
H	-0.1464820	-1.9775370	0.9002429	H	-0.4572510	-2.9307207	0.7387050	H	0.8496239	-3.2603411	1.2888291
H	3.0633831	-4.1090035	-0.9974042	H	2.6985215	-2.7136952	-2.1931389	H	1.8397976	-2.0110935	-2.7155459
H	2.5951956	-6.0950900	0.4321789	H	2.2798184	-5.0806491	-2.8083661	H	1.2695443	-4.2766484	-3.5576755
C	1.8237348	-1.6820394	-1.0150605	C	1.4025109	-1.1868165	-0.4411572	C	1.7133278	-1.0374914	-0.2220690
C	0.5992325	-1.0029489	-1.6298869	C	0.4361092	-0.1185505	-0.5305500	C	0.5585554	-0.0757479	-0.4144824
C	-0.5007952	-1.7561283	-2.0563184	C	-0.9438316	-0.2762650	-0.2563922	C	-0.7494432	-0.4255649	-0.0550603
C	0.5671205	0.3743408	-1.8577677	C	0.8899035	1.1960352	-0.8198592	C	0.7915077	1.2469627	-0.8169011
C	-1.6276548	-1.1776860	-2.6652336	C	-1.8277149	0.7912980	-0.2175062	C	-1.8052068	0.4910595	-0.0618768
H	-0.4921515	-2.8380397	-1.9121173	H	-1.3345702	-1.2759163	-0.0695767	H	-0.9500680	-1.4582966	0.2406562
C	-0.5256193	1.0031092	-2.4730244	C	0.0501037	2.2987411	-0.8387743	C	-0.2210730	2.2124216	-0.8617879
H	1.4186548	0.9845766	-1.5521937	H	1.9475701	1.3324757	-1.0634185	H	1.8038239	1.5314657	-1.1210563
C	-1.6359652	0.2210187	-2.8635829	C	-1.3688679	2.1545690	-0.5034433	C	-1.5872787	1.8745647	-0.4753496
O	-2.7789305	0.7921398	-3.3782126	O	-2.1507010	3.1544742	-0.4386634	O	-2.5289904	2.7463932	-0.4663998
C	-0.5287877	2.4788958	-2.6483239	C	0.5995503	3.6340152	-1.1729499	C	0.1214672	3.5939151	-1.2678689
C	-0.2330631	3.3206067	-1.5581851	C	1.8411302	4.0505927	-0.6519687	C	1.3228609	4.1930715	-0.8308374

C	-0.8061787	3.0697954	-3.8983990	C	-0.0798241	4.5114390	-2.0437312	C	-0.7169295	4.3524634	-2.1140980
C	-0.2168180	4.7091508	-1.7120825	C	2.3948556	5.2866178	-1.0002775	C	1.6844527	5.4816852	-1.2360379
H	-0.0224436	2.8742978	-0.5841794	H	2.3594614	3.4080037	0.0608859	H	1.9680317	3.6475479	-0.1400212
C	-0.7972639	4.4608744	-4.0488796	C	0.4734160	5.7463810	-2.3941588	C	-0.3561882	5.6403435	-2.5208353
H	-0.9944757	2.4347274	-4.7672602	H	-1.0470736	4.2128824	-2.4466552	H	-1.6572779	3.9168242	-2.4488541
C	-0.5039367	5.2847722	-2.9566667	C	1.7143643	6.1412826	-1.8760399	C	0.8468726	6.2140703	-2.0864886
H	0.0139292	5.3455790	-0.8557403	H	3.3560262	5.5871872	-0.5776867	H	2.6183629	5.9194986	-0.8764575
H	-1.0068648	4.8997604	-5.0260049	H	-0.0660785	6.4049113	-3.0784670	H	-1.0178567	6.2009399	-3.1852745
H	-0.4952473	6.3696572	-3.0746733	H	2.1428749	7.1079791	-2.1476213	H	1.1241297	7.2218756	-2.4018320
C	-2.7788887	-2.0381268	-3.0410335	C	-3.2366450	0.5428488	0.1662516	C	-3.1369929	0.0438034	0.4045650
C	-3.4187175	-1.9199876	-4.2906403	C	-4.3147199	1.1618801	-0.4999101	C	-4.3320957	0.4553389	-0.2251725
C	-3.2319472	-3.0326195	-2.1511727	C	-3.5322320	-0.3524752	1.2164018	C	-3.2460363	-0.8383940	1.5030548
C	-4.4710696	-2.7712344	-4.6385983	C	-5.6359419	0.8785781	-0.1416503	C	-5.5751597	-0.0118997	0.2121526
H	-3.0814630	-1.1590834	-4.9946217	H	-4.1052950	1.8656269	-1.3044525	H	-4.2719748	1.1487411	-1.0626279
C	-4.2857968	-3.8832405	-2.4986041	C	-4.8539862	-0.6344491	1.5755762	C	-4.4892020	-1.3056388	1.9406493
H	-2.7600586	-3.1289167	-1.1711175	H	-2.7103987	-0.8177822	1.7668103	H	-2.3395915	-1.1468366	2.0299012
C	-4.9102264	-3.7567266	-3.7450799	C	-5.9138868	-0.0207379	0.8966780	C	-5.6634577	-0.8956448	1.2964686
H	-4.9481594	-2.6679370	-5.6152595	H	-6.4557654	1.3609727	-0.6784497	H	-6.4836887	0.3137389	-0.2998403
H	-4.6237058	-4.6425810	-1.7906680	H	-5.0562196	-1.3280082	2.3945531	H	-4.5416843	-1.9839569	2.7952252
H	-5.7342385	-4.4186604	-4.0175811	H	-6.9466836	-0.2364576	1.1770779	H	-6.6358839	-1.2551793	1.6386850
O	0.7775148	-6.3003884	2.2129215	O	0.5016080	-6.6196590	-1.8205607	O	0.4447948	-6.2571295	-2.1764396
C	-0.2818002	-6.3057987	3.1870460	C	-0.5236967	-7.4117213	-1.1869967	C	-0.0134440	-7.3073875	-1.3037085
H	-1.2646295	-6.1571398	2.7112255	H	-1.5213519	-6.9756388	-1.3520339	H	-0.9547175	-7.0285593	-0.8037072
H	-0.2484178	-7.2959806	3.6541057	H	-0.4696584	-8.3957967	-1.6638197	H	-0.1853910	-8.1738699	-1.9509029
H	-0.1238430	-5.5318377	3.9554277	H	-0.3360058	-7.5144859	-0.1067214	H	0.7472549	-7.5581667	-0.5472076
H	2.4176553	-2.0678753	-1.8611480	H	2.3793476	-0.8990863	-0.8447613	H	2.5440938	-0.7028360	-0.8624900
C	2.7667922	-0.7403957	-0.2916097	C	2.0959243	-1.2743347	1.5391233	C	2.3026181	-0.9307333	1.2739982
C	4.1150478	-0.6732608	-0.7321404	C	3.2134716	-0.3514969	1.4587452	C	3.3743133	0.1355924	1.2390348
C	2.3182669	0.0421509	0.8050139	C	0.9120709	-0.8975157	2.2947320	C	1.1926129	-0.6675162	2.2734669
N	4.9696307	0.2094206	-0.0119058	N	2.8949820	0.9889972	1.7266521	N	2.9698829	1.4072688	1.6098019
O	4.6344760	-1.3076072	-1.6890342	O	4.3649246	-0.6486518	1.0990761	O	4.5119185	-0.0731328	0.8234157
N	3.2970519	0.8857402	1.4142826	N	0.7579868	0.4778016	2.5021203	N	0.9663327	0.6661229	2.5759560
O	1.1587737	0.0823576	1.2823097	O	0.0200442	-1.6725181	2.6744037	O	0.4894484	-1.5457921	2.7645971
C	4.6168916	1.0059512	1.0526915	C	1.6955235	1.4621750	2.2367635	C	1.7720626	1.7449414	2.2363170
O	5.4188634	1.7632562	1.6313368	O	1.4925675	2.6555070	2.4609145	O	1.4838944	2.9016513	2.5160302
H	-2.6713899	1.7657402	-3.3707347	H	2.3647394	-2.3272175	1.5796448	H	2.7878291	-1.8793000	1.5310649
H	5.9379206	0.2626781	-0.3238412	H	3.6333487	1.6807969	1.6005658	H	3.6341432	2.1721320	1.4822310
H	2.9803737	1.4571085	2.1961131	H	-0.1241758	0.7931993	2.9040658	H	0.1349414	0.8879571	3.1247774

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$\ominus_{N-E}$			
C	0.9573731	-5.1524159	1.4732626
C	0.1785518	-3.9914385	1.6017404
C	0.4503145	-2.8822170	0.7913467
C	1.4859848	-2.8964139	-0.1524049
C	2.2497910	-4.0710343	-0.2686664
C	1.9991186	-5.1859628	0.5311941

H	-		
	0.6374827	-3.9382492	2.3215269
H	-		
	0.1464820	-1.9775370	0.9002429
H	-		
	3.0633831	-4.1090035	-0.9974042
H	-		
	2.5951956	-6.0950900	0.4321789
C	-		
	1.8237348	-1.6820394	-1.0150605
C	-		
	0.5992325	-1.0029489	-1.6298869
C	-		
	0.5007952	-1.7561283	-2.0563184
C	-		
	0.5671205	0.3743408	-1.8577677
C	-		
	1.6276548	-1.1776860	-2.6652336
H	-		
	0.4921515	-2.8380397	-1.9121173
C	-		
	0.5256193	1.0031092	-2.4730244
H	-		
	1.4186548	0.9845766	-1.5521937
C	-		
	1.6359652	0.2210187	-2.8635829
O	-		
	2.7789305	0.7921398	-3.3782126
C	-		
	0.5287877	2.4788958	-2.6483239
C	-		
	0.2330631	3.3206067	-1.5581851
C	-		
	0.8061787	3.0697954	-3.8983990
C	-		
	0.2168180	4.7091508	-1.7120825
H	-		
	0.0224436	2.8742978	-0.5841794
C	-		
	0.7972639	4.4608744	-4.0488796
H	-		
	0.9944757	2.4347274	-4.7672602
C	-		
	0.5039367	5.2847722	-2.9566667
H	-		
	0.0139292	5.3455790	-0.8557403
H	-		
	1.0068648	4.8997604	-5.0260049
H	-		
	0.4952473	6.3696572	-3.0746733
C	-		
	2.7788887	-2.0381268	-3.0410335
C	-		
	3.4187175	-1.9199876	-4.2906403
C	-		
	3.2319472	-3.0326195	-2.1511727
C	-		
	4.4710696	-2.7712344	-4.6385983
H	-		
	3.0814630	-1.1590834	-4.9946217
C	-		
	4.2857968	-3.8832405	-2.4986041
H	-		
	2.7600586	-3.1289167	-1.1711175
C	-		
	4.9102264	-3.7567266	-3.7450799
H	-		
	4.9481594	-2.6679370	-5.6152595
H	-		
	4.6237058	-4.6425810	-1.7906680
H	-		
	5.7342385	-4.4186604	-4.0175811
O	-		
	0.7775148	-6.3003884	2.2129215
C	-		
	0.2818002	-6.3057987	3.1870460
H	-		
	1.2646295	-6.1571398	2.7112255
H	-		
	0.2484178	-7.2959806	3.6541057
H	-		
	0.1238430	-5.5318377	3.9554277
H	-		
	2.4176553	-2.0678753	-1.8611480
C	-		
	2.7667922	-0.7403957	-0.2916097
C	-		
	4.1150478	-0.6732608	-0.7321404
C	-		
	2.3182669	0.0421509	0.8050139

N	4.9696307	0.2094206	-0.0119058
O	4.6344760	-1.3076072	-1.6890342
N	3.2970519	0.8857402	1.4142826
O	1.1587737	0.0823576	1.2823097
C	4.6168916	1.0059512	1.0526915
O	5.4188634	1.7632562	1.6313368
H	2.6713899	1.7657402	-3.3707347
H	5.9379206	0.2626781	-0.3238412
H	2.9803737	1.4571085	2.1961131

B + 6a											
N _O [⊖] +E				TS _O				N _O -E [⊖]			
C	-5.4665252	-0.9594610	-0.9813559	C	-5.4580048	-1.3603710	-0.9591362	C	-4.7294572	0.9948764	-2.3264346
C	-4.6321058	0.0188153	-0.4054501	C	-4.7950388	-1.0288915	0.2341300	C	-4.6073884	0.6547102	-0.9702223
C	-3.2507666	-0.1397432	-0.4418888	C	-3.4058566	-1.1685671	0.3119609	C	-3.4709208	-0.0344020	-0.5287255
C	-2.6482151	-1.2714648	-1.0457758	C	-2.6563755	-1.6352483	-0.7763645	C	-2.4512274	-0.3969170	-1.4161453
C	-3.5189737	-2.2665884	-1.5723971	C	-3.3386832	-1.9879806	-1.9552094	C	-2.5928906	-0.0595435	-2.7733316
C	-4.8937040	-2.1117433	-1.5592784	C	-4.7198544	-1.8462118	-2.0536311	C	-3.7130233	0.6300917	-3.2280124
H	-5.0519935	0.8924174	0.0903470	H	-5.3434260	-0.6695987	1.1034241	H	-5.3831626	0.9143681	-0.2515583
H	-2.6404987	0.6008919	0.0734090	H	-2.8999257	-0.9329999	1.2486224	H	-3.3935044	-0.3009929	0.5254911
H	-3.0887139	-3.1679831	-2.0135461	H	-2.7780387	-2.3694098	-2.8114344	H	-1.8108764	-0.3358138	-3.4844335
H	-5.5509648	-2.8739506	-1.9796332	H	-5.2471779	-2.1156687	-2.9699542	H	-3.8223596	0.8886532	-4.2823544
C	-1.2316616	-1.5232699	-1.1055086	C	-1.1685636	-1.7241826	-0.7425848	C	-1.1707070	-1.0598597	-0.9623901
C	-0.1368975	-0.6746606	-0.9914994	C	-0.3694306	-0.5020075	-0.8061649	C	-0.0892309	-0.1052367	-0.5437913
C	-0.2008722	0.7617064	-0.9491051	C	-0.8304960	0.7479289	-0.3372310	C	-0.2940972	0.8213577	0.4897178
C	1.1743569	-1.2724426	-0.9472138	C	0.9905350	-0.5996646	-1.1780094	C	1.1503104	-0.1021173	-1.1958282
C	0.9137858	1.5409758	-0.7847500	C	0.0072497	1.8496720	-0.2057035	C	0.6924057	1.7240716	0.8913690
H	-1.1618777	1.2528197	-1.0952931	H	-1.8890329	0.8604225	-0.0926426	H	-1.2691435	0.8531773	0.9827765
C	2.3274795	-0.5468367	-0.8029708	C	1.8838719	0.4586346	-1.0590910	C	2.1799292	0.7801375	-0.8529913
H	1.2335063	-2.3602147	-1.0321470	H	1.3508476	-1.5580240	-1.5632249	H	1.3083607	-0.7982522	-2.0262401
C	2.2540883	0.9200264	-0.6591398	C	1.4308813	1.7541749	-0.5450754	C	1.9972410	1.7471044	0.2268922
O	3.2712274	1.6146429	-0.4333063	O	2.2259269	2.7332001	-0.3832303	O	2.9313361	2.5402813	0.5961892
C	3.6419797	-1.2269502	-0.7526567	C	3.3086985	0.2497240	-1.4079985	C	3.4715012	0.6937037	-1.5714723
C	3.7981051	-2.4104300	-0.0069310	C	3.9519504	-0.9623114	-1.0786942	C	4.0154540	-0.5605235	-1.9260559
C	4.7486847	-0.7373295	-1.4740245	C	4.0637876	1.2299803	-2.0866862	C	4.1920162	1.8482992	-1.9492995
C	5.0168428	-3.0938911	0.0074849	C	5.2872646	-1.1942969	-1.4201334	C	5.2123551	-0.6600704	-2.6425837
H	2.9599781	-2.7713183	0.5897241	H	3.3995967	-1.7283686	-0.5325254	H	3.4995344	-1.4729568	-1.6184929
C	5.9674765	-1.4221465	-1.4612084	C	5.3987995	0.9980526	-2.4313680	C	5.3885416	1.7497475	-2.6650918
H	4.6469166	0.1804605	-2.0527001	H	3.5914036	2.1777213	-2.3403489	H	3.7996204	2.8256159	-1.6722516
C	6.1077138	-2.6033143	-0.7211126	C	6.0201169	-0.2134236	-2.0996039	C	5.9072713	0.4961942	-3.0178528
H	5.1189622	-4.0065972	0.5981898	H	5.7591160	-2.1397923	-1.1446496	H	5.6089751	-1.6451271	-2.8981241
H	6.8118113	-1.0328314	-2.0338337	H	5.9590900	1.7690347	-2.9650397	H	5.9201165	2.6595016	-2.9536434
H	7.0613633	-3.1345590	-0.7089773	H	7.0646347	-0.3889429	-2.3641394	H	6.8445912	0.4220115	-3.5726540
C	0.7858885	3.0138683	-0.7030873	C	-0.5480556	3.1239390	0.3073483	C	0.4063909	2.6526531	2.0094087
C	1.6386113	3.8719749	-1.4255340	C	-0.2089086	4.3656164	-0.2704717	C	0.8160331	4.0038530	1.9771618
C	-0.2246705	3.5819409	0.0979227	C	-1.4641500	3.1255503	1.3798821	C	-0.3200561	2.2167704	3.1390044

C	1.4696086	5.2576333	-1.3638049	C	-0.7798320	5.5541511	0.1934595	C	0.4957612	4.8793716	3.0186327
H	2.4280571	3.4463373	-2.0444898	H	0.5068412	4.3876881	-1.0911970	H	1.3900195	4.3582326	1.1223301
C	-0.3874684	4.9696425	0.1622858	C	-2.0356560	4.3140345	1.8455238	C	-0.6407237	3.0920559	4.1816866
H	-0.8602601	2.9228490	0.6947588	H	-1.7190656	2.1813996	1.8663937	H	-0.6233978	1.1696957	3.2072269
C	0.4566494	5.8127509	-0.5700903	C	-1.6966384	5.5366056	1.2533824	C	-0.2346343	4.4309679	4.1277829
H	2.1308753	5.9088311	-1.9389824	H	-0.5094185	6.5019747	-0.2772467	H	0.8159694	5.9223598	2.9632642
H	-1.1711178	5.3937698	0.7934577	H	-2.7393660	4.2854863	2.6801381	H	-1.2004570	2.7234556	5.0441127
H	0.3309116	6.8959619	-0.5193427	H	-2.1373993	6.4667605	1.6171452	H	-0.4790008	5.1157064	4.9422187
O	-6.8238239	-0.8964664	-1.0071917	O	-6.8115619	-1.2596368	-1.1497460	O	-5.7952553	1.6681826	-2.8682786
C	-7.4677643	0.2579114	-0.4210662	C	-7.6094086	-0.7656282	-0.0554715	C	-6.8604570	2.0611651	-1.9810805
H	-7.1567521	1.1822516	-0.9305522	H	-7.3131435	0.2580890	0.2226038	H	-6.4963470	2.7482046	-1.2008039
H	-8.5401329	0.0970030	-0.5682737	H	-8.6407613	-0.7618488	-0.4230845	H	-7.5921569	2.5773458	-2.6113129
H	-7.2470063	0.3271691	0.6547151	H	-7.5337576	-1.4261821	0.8226519	H	-7.3328165	1.1835665	-1.5117760
H	-0.9784225	-2.5768732	-1.2640179	H	-0.7870743	-2.4979082	-1.4193463	H	-0.8003039	-1.7128023	-1.7682850
O	-1.2692977	-3.3934549	1.9405974	O	-0.8860031	-2.5155568	0.7352113	O	-1.5745211	-1.9476173	0.1802888
C	-0.6208742	-2.3290342	2.1097188	C	0.3304739	-2.3555432	1.2343495	C	-0.6902720	-2.8113279	0.6781085
N	-1.3631172	-1.1117151	2.1241307	N	0.5660728	-1.1629688	1.9060191	N	-1.1474195	-3.3602675	1.8611029
C	0.7706064	-2.1881224	2.2978168	C	1.3376390	-3.2861458	1.1314400	C	0.5233445	-3.1907569	0.1603444
C	-0.8407164	0.1591722	2.1867888	C	1.7975529	-0.7773975	2.4139337	C	-0.4567693	-4.3103000	2.5995944
C	1.4005840	-0.9271774	2.4121522	C	2.6369798	-3.0207081	1.6813788	C	1.3250201	-4.1608003	0.8512277
H	1.3862045	-3.0839099	2.3214838	H	1.1637161	-4.2188204	0.6026855	H	0.9150777	-2.7661299	-0.7553685
N	0.5242295	0.1985031	2.3349282	N	2.7705238	-1.7539090	2.2949331	N	0.7610658	-4.6580803	2.0504371
O	-1.5477639	1.1824663	2.1123398	O	1.9923511	0.3223731	2.9353059	O	-0.8999380	-4.7873578	3.6474278
O	2.6228881	-0.6947234	2.5626143	O	3.6233247	-3.7782970	1.6358650	O	2.4360954	-4.5807490	0.4858867
H	-2.3638837	-1.1841883	1.9496640	H	-0.1491550	-0.4371210	1.8617043	H	-2.0564972	-3.0678238	2.2173067
H	0.9545934	1.1208940	2.3609997	H	3.6883958	-1.5215194	2.6740545	H	1.3058822	-5.3509521	2.5639921

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N [⊕] +E				TS _c				N-E [⊖]			
C	0.7647105	-5.4466866	-1.2835628	C	0.7247964	-5.3871179	-1.4461856	C	0.8827867	-5.1002481	-1.6923312
C	-0.0368057	-4.6745954	-0.4185552	C	-0.0099900	-4.7833703	-0.4112232	C	0.7425424	-4.8001281	-0.3305245
C	0.0620832	-3.2881070	-0.4350356	C	0.1770034	-3.4292060	-0.1246722	C	1.0129865	-3.5019708	0.1273028
C	0.9565122	-2.6202530	-1.3069963	C	1.0891389	-2.6421793	-0.8517138	C	1.4226880	-2.4885108	-0.7457606
C	1.7942192	-3.4267752	-2.1243021	C	1.8472257	-3.2808571	-1.8583326	C	1.5612175	-2.8118659	-2.1097929
C	1.6931169	-4.8078761	-2.1301560	C	1.6642334	-4.6251405	-2.1634475	C	1.2976417	-4.0931720	-2.5830397
H	-0.7169550	-5.1491651	0.2868914	H	-0.7178548	-5.3575749	0.1846443	H	0.4249393	-5.5579434	0.3842886
H	-0.5009497	-2.7247275	0.3089961	H	-0.3508491	-2.9963325	0.7246263	H	0.8858063	-3.2874538	1.1888442
H	2.5225292	-2.9432661	-2.7786623	H	2.5844195	-2.7042376	-2.4213608	H	1.8788756	-2.0399734	-2.8150702
H	2.3280595	-5.4174330	-2.7743507	H	2.2453007	-5.1049986	-2.9524563	H	1.4132934	-4.3355590	-3.6408120
C	1.1188561	-1.1912241	-1.3916380	C	1.3217419	-1.1996368	-0.6245883	C	1.6688412	-1.0464793	-0.3319485
C	0.2494331	-0.1477323	-1.0948485	C	0.3054564	-0.1857800	-0.6671752	C	0.4637314	-0.1510968	-0.5252275
C	-1.1156169	-0.3127153	-0.6810283	C	-1.0543035	-0.4198832	-0.3453621	C	-0.8158075	-0.5602862	-0.1289361
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N _O [⊖] +E				TS _O				N _O -E [⊖]	
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H	2.8886899	1.5529277	-1.0868064	H	2.2061282	-0.5961863	-1.5053605	H	2.2447282	-0.4663945	-1.5156793
O	1.9703232	-1.9917845	-1.9937827	O	2.3489082	-0.6708075	0.6788719	O	2.3689434	-0.5447753	0.6015627
C	0.9773655	-2.1466599	-1.2395123	C	2.4142937	0.6322344	0.8829718	C	2.3990215	0.7812154	0.8078960
N	1.2043984	-2.1312789	0.1706793	N	1.4782177	1.1928462	1.7545244	N	1.4965129	1.2903990	1.7287067
C	-0.3565832	-2.3563167	-1.6480339	C	3.3389226	1.4450194	0.2642986	C	3.2700170	1.6082379	0.1493783
C	0.2053078	-2.3041022	1.1212616	C	1.4337223	2.5638433	2.0106059	C	1.4075406	2.6635159	1.9803285
C	-1.4209200	-2.5634365	-0.7482393	C	3.3754271	2.8556286	0.4749146	C	3.2627980	3.0242074	0.3545580
H	-0.5619459	-2.4341915	-2.7134386	H	4.0602772	1.0031678	-0.4179018	H	3.9721329	1.1894922	-0.5662965
N	-1.0905702	-2.4361727	0.6403199	N	2.3854044	3.3527048	1.3722416	N	2.2934167	3.4850548	1.2898350
O	0.4455176	-2.3420403	2.3402508	O	0.5816736	3.0514857	2.7621663	O	0.5735660	3.1190976	2.7682349
O	-2.6098781	-2.8310459	-1.0663414	O	4.1795342	3.6414220	-0.0648093	O	4.0128609	3.8320874	-0.2227546
C	-2.1525412	-2.5272034	1.6450429	C	2.3048468	4.7936306	1.6357331	C	2.1634442	4.9244298	1.5467254
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H	-2.0937848	-3.4761422	2.1977924	H	1.3182942	5.1714491	1.3376880	H	1.1491186	5.2562528	1.2905479
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H	3.1714002	-2.8948972	0.3107239	H	-0.5446510	0.6322712	1.9647238	H	-0.4887935	0.6286027	1.9975554
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H	2.5838602	-1.9371726	1.7104007	H	0.4253325	0.5814632	3.4723580	H	0.5169401	0.6740273	3.4838856

N [⊖] +E				TS _C				N-E [⊖]			
C	0.5713347	-5.3293221	-1.1221863	C	0.5344808	-5.3442092	-1.0497857	C	0.8223007	-5.1090179	-1.1924620
C	-0.2723266	-4.4544615	-0.3687333	C	-0.2276638	-4.6146933	-0.0940032	C	0.5790286	-4.6438289	0.1248565
C	-0.1645557	-3.0837491	-0.4784371	C	-0.0008518	-3.2622058	0.1308259	C	0.8587776	-3.3259584	0.4926056
C	0.7896898	-2.4707070	-1.3407335	C	0.9861280	-2.5450679	-0.5781298	C	1.3795613	-2.3995415	-0.4221395
C	1.6724585	-3.3509114	-2.0299219	C	1.7663126	-3.2780760	-1.4963711	C	1.6102400	-2.8542109	-1.7311329
C	1.5694406	-4.7248310	-1.9451706	C	1.5462088	-4.6286830	-1.7468404	C	1.3371427	-4.1643129	-2.1195530
H	-0.9943194	-4.8638066	0.3354530	H	-0.9992192	-5.1141371	0.4899058	H	0.1670613	-5.3127942	0.8788110
H	-0.7753267	-2.4719071	0.1833206	H	-0.5661817	-2.7638609	0.9176827	H	0.6498755	-3.0166661	1.5176822
H	2.4504692	-2.9207455	-2.6649454	H	2.5586659	-2.7665612	-2.0488038	H	2.0054895	-2.1592921	-2.4771526
H	2.2679705	-5.3410743	-2.5079890	H	2.1682789	-5.1295721	-2.4867906	H	1.5343421	-4.4519100	-3.1510774
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H	-1.5653185	-6.9228364	-0.3906954	H	-1.7907601	-6.9112478	-0.9938611	H	-1.2345798	-6.8945895	-0.5257293
H	-0.5378343	-8.3692434	-0.2837826	H	-0.8194252	-8.4071120	-0.9354392	H	-0.2585943	-8.2830594	-1.0878463
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H	1.3449559	-7.3701854	-2.8339510	H	0.7571105	-6.9377805	-3.3473833	H	-0.2295742	-6.2506137	-3.5292479
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C	0.1634422	0.0325605	-1.2210659	C	0.2912741	-0.0492985	-0.5581287	C	0.4642423	-0.0268615	-0.4163801
C	-1.1961140	-0.0382034	-0.7760144	C	-1.0807852	-0.2023435	-0.2574822	C	-0.8397949	-0.3704553	-0.0385139
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H	-1.6752209	-1.0117440	-0.6926650	H	-1.4535558	-1.1902310	0.0091139	H	-1.0177974	-1.3716299	0.3608204
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O	-2.0259118	3.4629882	-0.3781213	O	-2.3426527	3.1900837	-0.6838107	O	-2.6920327	2.6933064	-0.8002104
C	0.6142356	3.8236167	-1.4443699	C	0.3852635	3.6393232	-1.5054537	C	-0.0594167	3.5150171	-1.6689345
C	1.9213436	4.0953020	-0.9991657	C	1.6315458	4.1181820	-1.0540463	C	1.1179770	4.1950095	-1.2899564
C	-0.0728436	4.8258459	-2.1582305	C	-0.3254839	4.4267237	-2.4359232	C	-0.9055490	4.1470167	-2.6065701
C	2.5335435	5.3220330	-1.2753926	C	2.1599379	5.3241425	-1.5254350	C	1.4512125	5.4379727	-1.8369186
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C	0.5396183	6.0509802	-2.4361987	C	0.2017089	5.6317939	-2.9089378	C	-0.5737950	5.3894442	-3.1547803
H	-1.0893086	4.6344541	-2.5021047	H	-1.2969352	4.0810661	-2.7877763	H	-1.8286487	3.6491070	-2.9000552
C	1.8464345	6.3047720	-1.9978898	C	1.4482027	6.0879997	-2.4582853	C	0.6069971	6.0434536	-2.7759780
H	3.5464044	5.5152372	-0.9156785	H	3.1257288	5.6738765	-1.1540409	H	2.3671722	5.9413558	-1.5192552
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H	2.3217001	7.2638890	-2.2124858	H	1.8561449	7.0316267	-2.8257812	H	0.8614563	7.0158018	-3.2023327
C	-3.3421869	0.9243486	-0.0227189	C	-3.3790949	0.6121032	0.1422388	C	-3.2396590	0.0851148	0.3648207
C	-4.3970614	1.7103140	-0.5283618	C	-4.4813634	1.1980331	-0.5157349	C	-4.4487538	0.4288946	-0.2796800
C	-3.6362475	-0.0491620	0.9537237	C	-3.6416303	-0.2413418	1.2361630	C	-3.3249329	-0.7067659	1.5327439
C	-5.7078434	1.5138165	-0.0845681	C	-5.7899879	0.9252952	-0.1061809	C	-5.6800826	-0.0151655	0.2120776
H	-4.1842759	2.4715644	-1.2782647	H	-4.2995579	1.8692300	-1.3537596	H	-4.4082159	1.0522833	-1.1712907
C	-4.9481353	-0.2408878	1.3984898	C	-4.9502877	-0.5129850	1.6463560	C	-4.5558868	-1.1506006	2.0244559

H	-2.8180524	-0.6306799	1.3880884	H	-2.8034839	-0.6841923	1.7795320	H	-2.4093291	-0.9638552	2.0700124
C	-5.9902597	0.5378532	0.8806054	C	-6.0334978	0.0693114	0.9763975	C	-5.7439066	-0.8073286	1.3664186
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H	-7.0141493	0.3903323	1.2296311	H	-7.0563868	-0.1375490	1.2969932	H	-6.7072766	-1.1479792	1.7509699
H	1.9292202	-0.8085992	-1.9900351	H	2.2343854	-0.8404929	-0.8611972	H	2.4764989	-0.6234411	-0.7524294
C	1.3442643	-1.5113130	1.8689367	C	1.9829336	-1.0284163	1.5453837	C	2.1817204	-0.6994643	1.3941227
C	2.5172841	-0.9188313	1.3642100	C	3.1509557	-0.1917566	1.3677336	C	3.2571522	0.3465277	1.2979200
C	0.2014734	-0.7797641	2.2356455	C	0.8383423	-0.5320532	2.2843389	C	1.0519962	-0.3497896	2.3302687
N	2.5472637	0.5117580	1.3712468	N	2.9464468	1.1903677	1.5235929	N	2.8549119	1.6619671	1.4741699
O	3.5220057	-1.5287009	0.9146945	O	4.2659605	-0.6134515	1.0123614	O	4.4151615	0.0747711	0.9758977
N	0.3453416	0.6477433	2.2175481	N	0.7376292	0.8682857	2.3640869	N	0.7652054	1.0075907	2.4480075
O	-0.9110649	-1.2737669	2.5680788	O	-0.0632653	-1.2570665	2.7387016	O	0.3760512	-1.2029657	2.9040411
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H	1.2670750	-2.5943455	1.8310439	H	2.1990492	-2.0847119	1.6877201	H	2.6485855	-1.6272844	1.7420753
C	3.7537449	1.1681155	0.8679008	C	4.0714293	2.0788139	1.2058757	C	3.8294835	2.7192932	1.1607946
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H	4.6340214	0.6113349	1.2062803	H	4.9572568	1.7676215	1.7717446	H	4.7218963	2.5922322	1.7846906
H	3.7566988	1.1857284	-0.2324299	H	4.2991535	2.0222842	0.1331790	H	4.1168553	2.6491446	0.1043400
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H	-1.0180165	2.2299741	1.9129458	H	-0.8906959	2.1584017	2.0590287	H	-1.1397575	1.8741078	2.2519568

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N-E

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C	-1.9813947	-4.2729838	1.4559974
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H	1.0339359	-1.1222084	6.0157649
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H	2.6867589	0.6729026	6.5427910
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H	-0.9296820	4.6542826	0.3975377
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C	-2.0802602	-6.7643576	2.8500158
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H	4.4789089	-0.5614103	-2.4669366
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H	-0.4638530	-0.4383786	-5.7727227
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H	-0.6933305	-7.9633621	0.0263012
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H	-0.9346794	-8.6856493	1.6242463

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$N_o^{\ominus} + E$				TS_o				$N_o - E^{\ominus}$			
C	0.0791059	1.1394817	-5.1827727	C	-5.3808602	0.6260395	-1.6160355	C	-5.2982270	0.6877764	-1.7132860
C	-0.8373932	0.5738105	-4.2439261	C	-4.6134165	1.7337343	-2.0683630	C	-4.5092137	1.8300960	-2.0156929
C	-0.6119157	0.6510322	-2.8874561	C	-3.2212189	1.7036131	-2.0316580	C	-3.1170408	1.7689266	-1.9864252
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C	1.2435446	1.7771653	-4.6590314	C	-4.6638157	-0.4961536	-1.1156170	C	-4.6037688	-0.5015141	-1.3621566
H	-1.7170570	0.0373231	-4.5942414	H	-5.1042581	2.6228030	-2.4603693	H	-4.9821988	2.7730014	-2.2845808
H	-1.3086048	0.1404745	-2.2288921	H	-2.6666230	2.5719275	-2.3963617	H	-2.5457556	2.6680741	-2.2312159
H	2.3685857	2.3111826	-2.9299478	H	-2.7599374	-1.3884804	-0.7058826	H	-2.7155203	-1.4735402	-1.0666114
H	1.9858713	2.2074795	-5.3284999	H	-5.1962122	-1.3772376	-0.7614851	H	-5.1527786	-1.4084719	-1.1148124
C	0.8863420	1.3994223	-0.9751405	C	-1.0370797	0.6409259	-1.4386071	C	-0.9460265	0.5948499	-1.5345926
C	0.2099891	1.1300739	0.2239435	C	-0.3583897	0.6762882	-0.1391248	C	-0.3340699	0.6495045	-0.1811434
C	-1.1653822	0.7531262	0.3579180	C	-0.9372070	0.2062795	1.0571333	C	-0.9669898	0.1455520	0.9681654
C	0.9584620	1.2678589	1.4408441	C	0.9900673	1.0928546	-0.0881536	C	0.9970634	1.0892100	-0.0514400
C	-1.7525730	0.5147572	1.5781409	C	-0.2190229	0.0983184	2.2430574	C	-0.3155012	0.0379144	2.1957589
H	-1.7948463	0.6932562	-0.5275829	H	-1.9943546	-0.0648204	1.0599640	H	-2.0130453	-0.1605037	0.9006984
C	0.4302276	1.0356087	2.6888173	C	1.7701564	1.0029784	1.0611878	C	1.7148592	0.9957517	1.1412150
H	2.0084742	1.5601631	1.3579228	H	1.4345780	1.5043262	-0.9990711	H	1.4859435	1.5205265	-0.9300369
C	-0.9763120	0.6299262	2.8263784	C	1.1974937	0.4688595	2.2992285	C	1.0833991	0.4432857	2.3401877
O	-1.4867415	0.3583998	3.9449291	O	1.8911676	0.3146662	3.3571681	O	1.7189815	0.2974608	3.4386983
C	1.2898236	1.1284333	3.8922089	C	3.1907235	1.4199506	1.0073680	C	3.1324578	1.4235555	1.1645012
C	2.5830836	0.5683280	3.8749278	C	3.9621911	1.1775806	-0.1494801	C	3.9655779	1.1932541	0.0479230
C	0.8554971	1.7812963	5.0633144	C	3.8176439	2.0905974	2.0800702	C	3.7003461	2.0880302	2.2736632
C	3.4226160	0.6725796	4.9891373	C	5.2934147	1.5918776	-0.2414018	C	5.2976172	1.6146562	0.0284000
H	2.9091321	0.0236768	2.9856425	H	3.5119717	0.6418882	-0.9854854	H	3.5627461	0.6608019	-0.8142271
C	1.6975357	1.8872740	6.1739400	C	5.1495078	2.5067355	1.9895963	C	5.0330882	2.5109076	2.2558207
H	-0.1453749	2.2109212	5.0946800	H	3.2475155	2.2805826	2.9879180	H	3.0825803	2.2665532	3.1521645
C	2.9849984	1.3342206	6.1427583	C	5.8975338	2.2602400	0.8306035	C	5.8418663	2.2774933	1.1354716
H	4.4194218	0.2272619	4.9589585	H	5.8628866	1.3856572	-1.1501278	H	5.9149935	1.4176049	-0.8506788
H	1.3483446	2.4060817	7.0692077	H	5.6074329	3.0312331	2.8312863	H	5.4440687	3.0305731	3.1243879
H	3.6387445	1.4143008	7.0134626	H	6.9388585	2.5812912	0.7656566	H	6.8835617	2.6038180	1.1273680
C	-3.1782249	0.1170374	1.6454258	C	-0.8938848	-0.4363059	3.4490552	C	-1.0457932	-0.5368931	3.3493671
C	-4.0761197	0.7519775	2.5261292	C	-0.6954871	0.1314547	4.7256795	C	-0.9313911	0.0043084	4.6481050
C	-3.6663721	-0.8956004	0.7969809	C	-1.7845707	-1.5257726	3.3457108	C	-1.9065301	-1.6416668	3.1734251
C	-5.4288863	0.4011364	2.5383097	C	-1.3761168	-0.3578130	5.8441997	C	-1.6626094	-0.5243006	5.7157203
H	-3.7076936	1.5296562	3.1952563	H	-0.0009897	0.9640530	4.8300184	H	-0.2608547	0.8472961	4.8093292
C	-5.0204510	-1.2478688	0.8140502	C	-2.4659858	-2.0165765	4.4642146	C	-2.6385739	-2.1717036	4.2408168
H	-2.9617967	-1.4384946	0.1617146	H	-1.9311904	-2.0043882	2.3749062	H	-1.9891495	-2.1011311	2.1859657
C	-5.9079840	-0.5986550	1.6805820	C	-2.2658101	-1.4339961	5.7215020	C	-2.5212886	-1.6148479	5.5201559
H	-6.1139966	0.9110776	3.2188257	H	-1.2135097	0.1057291	6.8198339	H	-1.5643484	-0.0800715	6.7088686
H	-5.3815034	-2.0402171	0.1547866	H	-3.1468910	-2.8633800	4.3545052	H	-3.2940413	-3.0293293	4.0743067

H	-6.9642690	-0.8744286	1.6949535	H	-2.7925086	-1.8172855	6.5975797	H	-3.0876076	-2.0288400	6.3566804
C	-1.3259086	0.3690027	-7.0441100	C	-7.4628784	1.8688926	-1.9998323	C	-7.3545228	2.0158515	-1.8967897
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H	-1.3367315	0.4589891	-8.1340975	H	-8.5386738	1.6673039	-2.0362761	H	-8.4342985	1.8460909	-1.9681712
H	-1.3134774	-0.7016208	-6.7838057	H	-7.2797748	2.6603867	-1.2497928	H	-7.1592069	2.6745931	-1.0299207
H	1.9040394	1.7759090	-0.8210742	H	-0.6113314	1.3684443	-2.1412286	H	-0.5153678	1.3692112	-2.1858229
N	-0.1448284	1.0602692	-6.5244218	N	-6.7608679	0.6285029	-1.6809005	N	-6.6811628	0.7248372	-1.7794576
C	0.8336198	1.5929991	-7.4735172	C	-7.5147950	-0.4238205	-1.0040464	C	-7.4515427	-0.3812854	-1.2160389
H	0.9976669	2.6695967	-7.3127082	H	-7.2459129	-1.4165263	-1.3945277	H	-7.1971259	-1.3306169	-1.7095566
H	1.8010894	1.0725945	-7.3886044	H	-7.3482092	-0.4235861	0.0888960	H	-7.2870190	-0.4999403	-0.1287238
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O	1.8769823	-1.5586761	-3.3066931	O	-0.5981289	-0.8054588	-2.2166089	O	-0.5054308	-0.7612697	-2.2405426
C	1.4664159	-1.7513879	-2.1368613	C	0.7075741	-0.9599514	-2.3783467	C	0.8187579	-0.9134930	-2.3686481
N	2.3228362	-1.3879323	-1.0409199	N	1.3681891	-1.7915756	-1.4747350	N	1.4397685	-1.7749636	-1.4753470
C	0.2199825	-2.2964315	-1.7703202	C	1.4189646	-0.3312138	-3.3747370	C	1.5479434	-0.2583745	-3.3271454
C	2.0330754	-1.6427611	0.2899396	C	2.7482291	-1.9938213	-1.5306115	C	2.8242173	-1.9700053	-1.4898991
C	-0.1803731	-2.5064293	-0.4379598	C	2.8305456	-0.4882450	-3.5158501	C	2.9666739	-0.4072345	-3.4271010
H	-0.4755509	-2.5594500	-2.5635597	H	0.8961132	0.3180891	-4.0718279	H	1.0448225	0.4106646	-4.0198591
N	0.7719588	-2.1434042	0.5699322	N	3.4363652	-1.3445978	-2.5508074	N	3.5426322	-1.2855266	-2.4654639
O	2.8721852	-1.4184683	1.1843264	O	3.3285431	-2.7080982	-0.7053826	O	3.3782472	-2.7054776	-0.6671682
O	-1.2806157	-2.9951182	-0.0649436	O	3.5300074	0.0638831	-4.3878620	O	3.6882527	0.1709365	-4.2607015
C	0.4136309	-2.3650772	1.9713489	C	4.8889428	-1.5493398	-2.5750262	C	4.9970365	-1.4816360	-2.4445565
H	0.9793847	-1.6672321	2.5940741	H	5.1179563	-2.6126578	-2.7180776	H	5.2367748	-2.5394327	-2.6084063
H	-0.6596310	-2.1826520	2.0812451	H	5.2916569	-0.9612647	-3.4035811	H	5.4248362	-0.8691223	-3.2421419
H	0.6371516	-3.3972941	2.2813072	H	5.3269472	-1.2158878	-1.6253970	H	5.3988000	-1.1720200	-1.4712225
C	3.6136849	-0.7639284	-1.3275067	C	0.6650964	-2.4357675	-0.3573868	C	0.7025095	-2.4491960	-0.3967577
H	3.5807484	-0.4158115	-2.3640519	H	-0.4066165	-2.2970118	-0.5073825	H	-0.3649601	-2.3312737	-0.5873770
H	3.7731295	0.0789619	-0.6448140	H	0.9164592	-3.5018457	-0.3340846	H	0.9760149	-3.5095686	-0.3808816
H	4.4411551	-1.4779220	-1.2036010	H	0.9627250	-1.9637673	0.5883553	H	0.9518305	-1.9849100	0.5665031

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