

Supporting Information

for

Pd(II)-Catalyzed Aerobic Dual C–N Bond Formation: Oxygen-Dependent Divergence between Dihydroquinazolinone and Aza-Michael Pathways, an Experimental and Computational Study

Narges Mohammadi,^a Farnaz Jafarpour,^{*,a} Leyla Mohammadkhani,^b Alireza Ariafard^{*,c}

^a School of Chemistry, College of Science, University of Tehran, 14155-6455 Tehran, Iran

^b Department of Chemistry, Islamic Azad University, Central Tehran Branch, Poonak, Tehran, 1419953491, Iran

^c Research School of Chemistry, Australian National University, Canberra, Acton ACT 2601, Australia

Author Information

Corresponding Authors

*E-mail: Jafarpour@ut.ac.ir

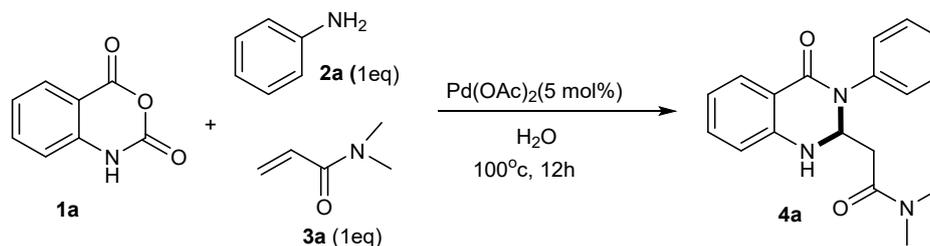
*E-mail: Alireza.Ariafard@anu.edu.au

Contents

1. General remarks.....	3
2. General experimental procedure for synthesis of 2,3-Dihydroquinazolin-4(1 <i>H</i>)-one.....	3
3. Crystallographic details	4
4. Experimental characterization data.....	6
5. Copies of ¹ H and ¹³ C NMR spectra of products	8
6. Computational details	18
Mechanism of anthranilamide formation from isatoic anhydride and aniline.....	18
Solvent effects on the formation of anthranilamide 5	19
Substituent effects on the formation of anthranilamide 5	20
Formation of the Pd(II)–hydroperoxo species:.....	21
7. Total energies for all of the calculated structures	23
8. Cartesian coordinates for all of the calculated structures	24
9. References.....	70

1. General remarks

The following includes general experimental procedures, specific details for representative reactions and spectroscopic information for new compounds. Palladium catalysts were commercially available and used as received. Unless otherwise noted, all other reagents and starting materials were purchased from Merck company and other commercial sources. Unless noted, all commercial reagents were used without further purification. The reactions were carried out in oil bath using microwave vials (2-5 mL). Melting points were measured with an Electrothermal 9100 apparatus. ^1H NMR spectra were recorded at room temperature on Varian-INOVA 500MHz and Bruker DRX400 MHz spectrometers, using CDCl_3 as the NMR solvent, except in one case where DMSO-d_6 was used. ^1H NMR spectra are referenced to tetramethylsilane (0.00 ppm) and ^{13}C NMR spectra are referenced from the solvent central peak (77.23 ppm for CDCl_3 and 39.52 ppm for DMSO-d_6). Chemical shifts are given in ppm. IR spectra were measured with a Bruker- Equinox 55. Mass spectra were recorded on a FINNIGAN-MAT 8430 mass spectrometer operating at an ionization potential of 70 eV. Crystallographic data were collected on a MAR345 dtb diffractometer equipped with an image plate detector using $\text{Mo-K}\alpha$ X-ray radiation. The structures were solved by direct methods using SHELXS-2013 and refined using full-matrix least-squares method on F^2 , SHELXL-2016.



Scheme S1. Substrate scope

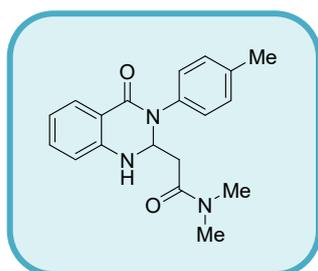
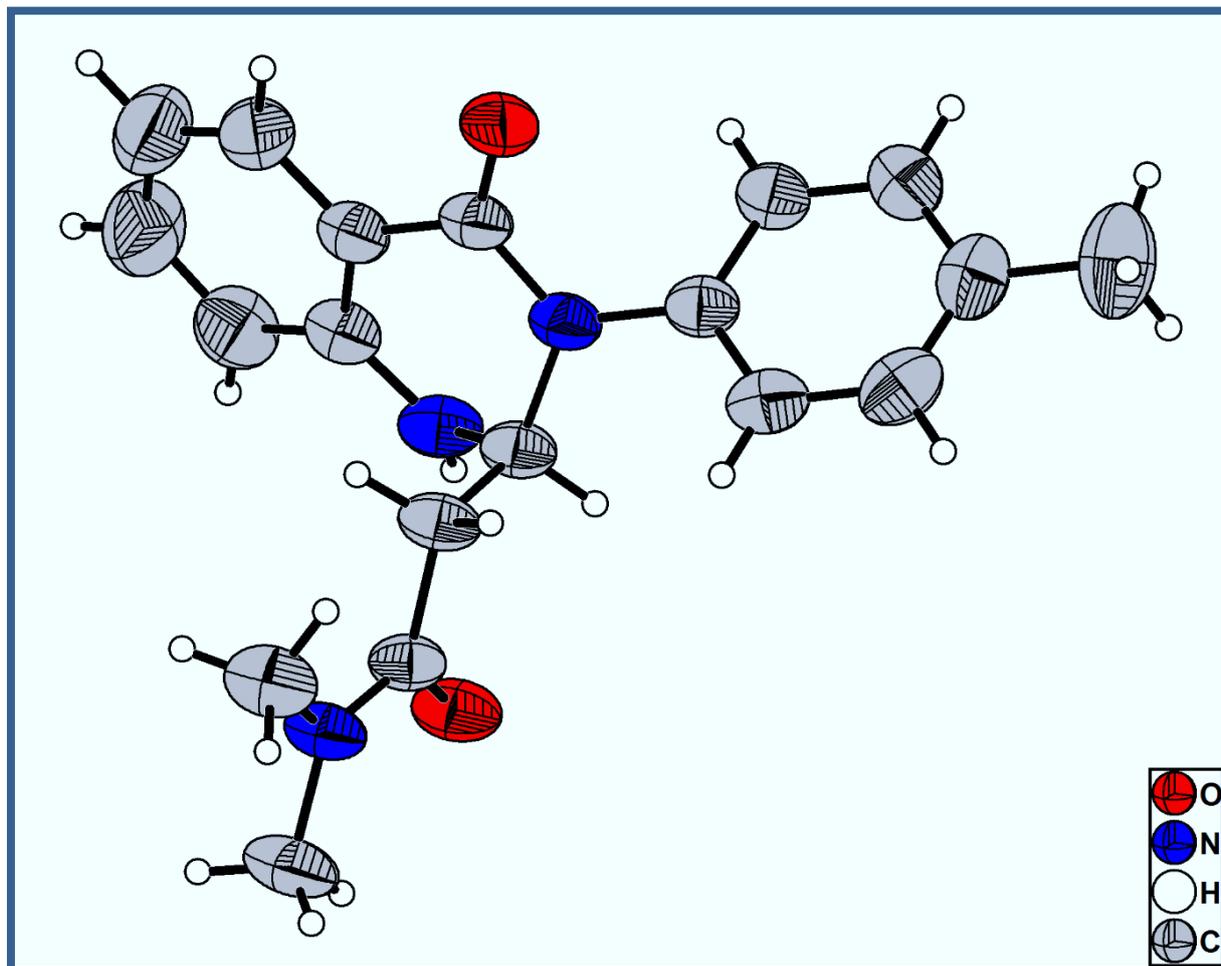
2. General experimental procedure for synthesis of 2,3-Dihydroquinazolin-4(1H)-one

A vial equipped with a stir bar was charged with, isatoic anhydride (0.1 mmol, 1 equiv), aniline (0.1 mmol, 1 equiv), acrylamide (0.5 mmol, 5 equiv), $\text{Pd}(\text{OAc})_2$ (5 mol%), and H_2O (1 mL) was added and the vial was capped. The resulting mixture was heated in an oil bath at 100°C for 12 h under air. After cooling, the reaction mixture was poured into water and extracted with EtOAc. cooled then filtered through a short plug of silica. The residue was purified by flash column chromatography (silica gel, hexane/EtOAc) to give desired product 3.

3. Crystallographic details

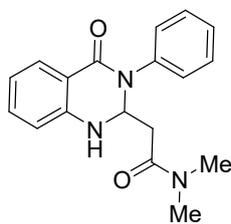
Compound **4c** was dissolved in ethyl acetate and some drops of hexane were added and the formation and growth of crystals were monitored over a few days while the solvent was gradually evaporated.

Figure S1. Crystal structure of 6-chloro-2-(4-chlorophenyl)-1,3-diphenyl-1H-indole **4c** with atoms represented as thermal vibration ellipsoids of 50% probability.



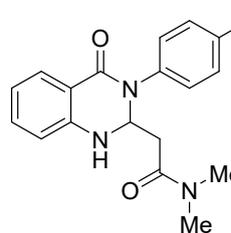
4. Experimental characterization data

N, N-dimethyl-2-(4-oxo-3-tetrahydroquinazolin-2-yl) acetamide (*4a*)

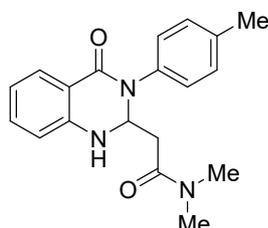


White solid (18.5 mg, yield 60%); mp 188-190 °C; IR (KBr) (cm⁻¹) 3269, 1652, 1617; ¹H NMR (400 MHz, CDCl₃) δ_H 7.99 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.53 – 7.41 (m, 4H), 7.40 – 7.30 (m, 2H), 6.89 (t, *J* = 7.4 Hz, 1H), 6.73 (d, *J* = 8.0 Hz, 1H), 5.55 (dd, *J* = 10.2, 2.1 Hz, 1H), 3.09 (dd, *J* = 16.6, 10.2 Hz, 1H), 2.91 (s, 3H), 2.86 (s, 3H), 2.68 (dd, *J* = 16.6, 2.1 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ_C 169.9, 162.2, 145.6, 140.2, 133.9, 129.3, 129.0, 127.2, 127.1, 119.0, 115.7, 115.3, 69.9, 36.9, 35.0. Anal. Calcd for C₁₈H₁₉N₃O₂: C, 69.88; H, 6.19; N, 13.58; Found: C, 69.65; H, 6.08; N, 13.40.

2-(3-(4-methoxyphenyl)-4-oxo-1,2,3,4-tetrahydroquinazolin-2-yl)-N, N-dimethylacetamide (*4b*)

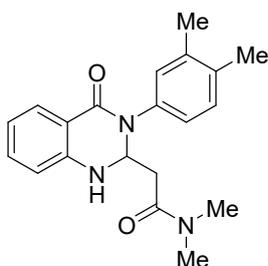


White solid (18.6 mg, yield 55%); mp 194-196 °C; ¹H NMR (400 MHz, CDCl₃) δ_H 7.98 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.39 – 7.29 (m, 2H), 6.97 (d, *J* = 6.6 Hz, 1H), 6.87 (t, *J* = 7.0 Hz, 1H), 6.71 (d, *J* = 8.2 Hz, 1H), 5.47 (dd, *J* = 10.2, 2.1 Hz, 1H), 3.84 (s, 3H), 3.05 (dd, *J* = 16.6, 10.2 Hz, 1H), 2.91 (s, 3H), 2.87 (s, 3H), 2.75 – 2.64 (m, 1H); ¹³C NMR (101 MHz, CDCl₃) δ_C 169.0, 162.4, 158.4, 145.7, 133.8, 132.9, 128.9, 128.6, 118.9, 115.7, 115.2, 114.6, 70.1, 55.5, 36.9, 35.0. Anal. Calcd for C₁₉H₂₁N₃O₃: C, 67.24; H, 6.24; N, 12.38; Found: C, 67.49; H, 6.36; N, 12.58.



N, N-dimethyl-2-(4-oxo-3-(p-tolyl)-1,2,3,4-tetrahydroquinazolin-2-yl) acetamide (*4c*)

Cream solid (20.9 mg, yield 65%); mp 207-209 °C; ¹H NMR (400 MHz, CDCl₃) δ_H 7.98 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.36 – 7.28 (m, 3H), 7.24 (s, 1H), 6.87 (t, *J* = 7.7 Hz, 1H), 5.50 (dd, *J* = 10.2, 2.1 Hz, 1H), 3.06 (dd, *J* = 16.7, 10.2 Hz, 1H), 2.90 (s, 3H), 2.85 (s, 3H), 2.67 (dd, *J* = 16.5, 2.2 Hz, 1H), 2.38 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ_C 170.0, 162.2, 145.7, 137.6, 137.1, 133.8, 130.0, 129.0, 127.1, 119.0, 115.8, 115.2, 70.0, 36.9, 35.1, 21.1; MS *m/z* (%): 339 (M⁺, 2), 253 (100), 72 (20). Anal. Calcd for C₁₉H₂₁N₃O₂: C, 70.57; H, 6.55; N, 12.99; Found: C, 70.89; H, 6.64; N, 13.17.



2-(3-(3,4-dimethylphenyl)-4-oxo-1,2,3,4-tetrahydroquinazolin-2-yl)-N, N-dimethylacetamide (*4d*)

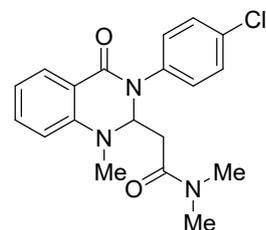
Cream solid (17.8 mg, yield 53%); mp 141-143 °C; ¹H NMR (499 MHz, CDCl₃) δ_H 7.96 (dt, *J* = 7.8, 1.4 Hz, 1H), 7.35 – 7.28 (m, 1H), 7.22 – 7.16 (m, 2H), 6.85 (t, *J* = 7.4 Hz, 1H), 6.69 (d, *J* = 8.0 Hz, 1H), 5.48 (dd, *J* = 10.1, 2.1 Hz, 1H), 3.04 (dd, *J* = 16.6, 10.2 Hz, 1H), 2.88 (s, 3H), 2.84 (d, *J* = 1.3 Hz, 3H), 2.66 (dd, *J* = 16.6, 2.2 Hz, 1H), 2.28 (s, 3H), 2.27 (s, 3H); ¹³C NMR (126 MHz, CDCl₃) δ_C 170.0, 162.2, 145.7, 137.9, 137.7, 135.8, 133.7, 130.4, 129.0, 128.4, 124.6, 118.9, 115.9, 115.2, 70.0, 36.9, 35.1, 35.0, 19.9, 19.4. Anal. Calcd for C₂₀H₂₃N₃O₂: C, 71.19; H, 6.87; N, 12.45; Found: C, 71.44; H, 6.99; N, 12.70.

2-(3-(5-methoxy-2-methylphenyl)-4-oxo-1,2,3,4-tetrahydroquinazolin-2-yl)-N,N-dimethylacetamide (4e)



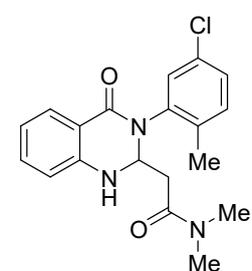
Cream solid (19.7 mg, yield 56%); mp 141-143 °C; ¹H NMR (400 MHz, CDCl₃) δ_H 8.06 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.44 – 7.35 (m, 1H), 7.22 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.00 (d, *J* = 8.3 Hz, 1H), 6.97 – 6.91 (m, 1H), 6.80 (d, *J* = 8.0 Hz, 1H), 5.47 (d, *J* = 10.1 Hz, 1H), 3.94 (s, 3H), 3.13 (dd, *J* = 16.7, 10.2 Hz, 1H), 2.99 (s, 3H), 2.94 (s, 3H), 2.77 (d, *J* = 16.5 Hz, 1H), 2.41 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ_C 170.3, 162.2, 145.9, 133.6, 129.6, 128.9, 118.7, 115.9, 115.2, 112.3, 56.0, 36.9, 35.4, 35.0, 20.4. Anal. Calcd for C₂₀H₂₃N₃O₃: C, 67.97; H, 6.56; N, 11.89; Found: C, 68.19; H, 6.66; N, 12.07.

2-(3-(4-chlorophenyl)-1-methyl-4-oxo-1,2,3,4-tetrahydroquinazolin-2-yl)-N,N-dimethylacetamide (4f)



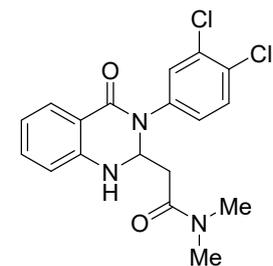
Yellow oil (21.4 mg, yield 60%); ¹H NMR (400 MHz, CDCl₃) δ_H 8.05 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.47 (ddd, *J* = 8.5, 7.2, 1.6 Hz, 1H), 6.99 – 6.90 (m, 1H), 6.76 (d, *J* = 8.2 Hz, 1H), 5.63 (dd, *J* = 8.2, 3.7 Hz, 1H), 3.11 (s, 3H), 3.05 (dd, *J* = 15.3, 8.3 Hz, 1H), 2.88 (s, 3H), 2.80 (s, 3H), 2.69 (dd, *J* = 15.3, 3.8 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ_C 168.9, 161.9, 146.3, 138.8, 134.3, 132.0, 129.4, 129.3, 127.0, 119.1, 117.5, 114.1, 76.4, 38.2, 37.4, 35.6, 34.9. Anal. Calcd for C₁₉H₂₀ClN₃O₂: C, 63.77; H, 5.63; N, 11.74; Found: C, 63.51; H, 5.50; N, 11.53.

2-(3-(5-chloro-2-methylphenyl)-4-oxo-1,2,3,4-tetrahydroquinazolin-2-yl)-N,N-dimethylacetamide (4g)



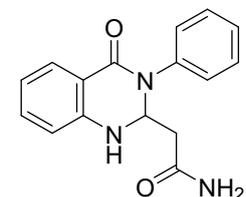
Cream solid (21.4 mg, yield 60%); mp 206-209 °C; ¹H NMR (499 MHz, CDCl₃) δ_H 7.95 (d, *J* = 7.9 Hz, 1H), 7.38 – 7.30 (m, 1H), 7.30 – 7.22 (m, 4H), 6.88 (t, *J* = 7.5 Hz, 1H), 6.72 (d, *J* = 8.1 Hz, 1H), 5.14 (d, *J* = 10.1 Hz, 1H), 3.13 (dd, *J* = 16.4, 10.1 Hz, 1H), 2.90 (s, 6H), 2.35 (s, 3H); ¹³C NMR (126 MHz, CDCl₃) δ_C 169.7, 162.1, 145.8, 139.7, 134.3, 134.0, 132.6, 131.4, 129.6, 128.9, 128.3, 119.0, 115.5, 115.3, 68.8, 36.9, 35.0, 34.9, 17.3. Anal. Calcd for C₁₉H₂₀ClN₃O₂: C, 63.77; H, 5.63; N, 11.74; Found: C, 64.06; H, 5.80; N, 11.98.

2-(3-(3,4-dichlorophenyl)-4-oxo-1,2,3,4-tetrahydroquinazolin-2-yl)-N,N-dimethylacetamide (4h)



White solid (21.6 mg, yield 60%); mp 187-190 °C; ¹H NMR (400 MHz, CDCl₃) δ_H 7.97 (d, *J* = 7.9 Hz, 1H), 7.61 (t, *J* = 2.2 Hz, 1H), 7.51 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.41 – 7.30 (m, 2H), 6.90 (t, *J* = 7.4 Hz, 1H), 6.72 (d, *J* = 8.1 Hz, 1H), 5.59 – 5.50 (m, 1H), 3.09 (dd, *J* = 16.5, 10.3 Hz, 1H), 2.92 (s, 3H), 2.88 (s, 3H), 2.61 (dd, *J* = 16.7, 2.3 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ_C 169.5, 162.1, 145.6, 139.5, 134.4, 133.0, 130.9, 130.8, 129.1, 129.0, 126.2, 119.3, 115.4, 115.2, 77.4, 77.3, 77.1, 76.7, 69.8, 60.4, 36.9, 35.1. Anal. Calcd for C₁₈H₁₇Cl₂N₃O₂: C, 57.16; H, 4.53; N, 11.11; Found: C, 57.47; H, 4.65; N, 11.39.

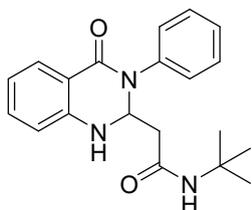
2-(4-oxo-3-phenyl-1,2,3,4-tetrahydroquinazolin-2-yl) acetamide (4i)



White solid (14.6mg, yield 52%); mp 155-158 °C; ¹H NMR (400 MHz, DMSO) δ_H 7.73 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.49 – 7.36 (m, 5H), 7.32 (m, 2H), 7.18 (d, *J* = 3.4 Hz, 1H), 6.97 (s, 1H), 6.89 (d, *J* = 8.2 Hz, 1H), 6.76 (t, *J* = 7.5 Hz, 1H), 5.44 (m, 1H), 2.77 (dd, *J* = 14.9, 9.4 Hz, 1H), 2.46 (m, 1H); ¹³C NMR (101 MHz,

DMSO) δ_C 170.9, 161.8, 146.9, 141.0, 134.1, 129.4, 128.4, 127.4, 127.0, 117.9, 115.9, 115.4, 69.5, 38.8; MS m/z (%): 281 (M^+ , 2), 223 (100), 77 (10). Anal. Calcd for $C_{16}H_{15}N_3O_2$: C, 68.54; H, 5.37; N, 14.94; Found: C, 68.31; H, 5.47; N, 15.09.

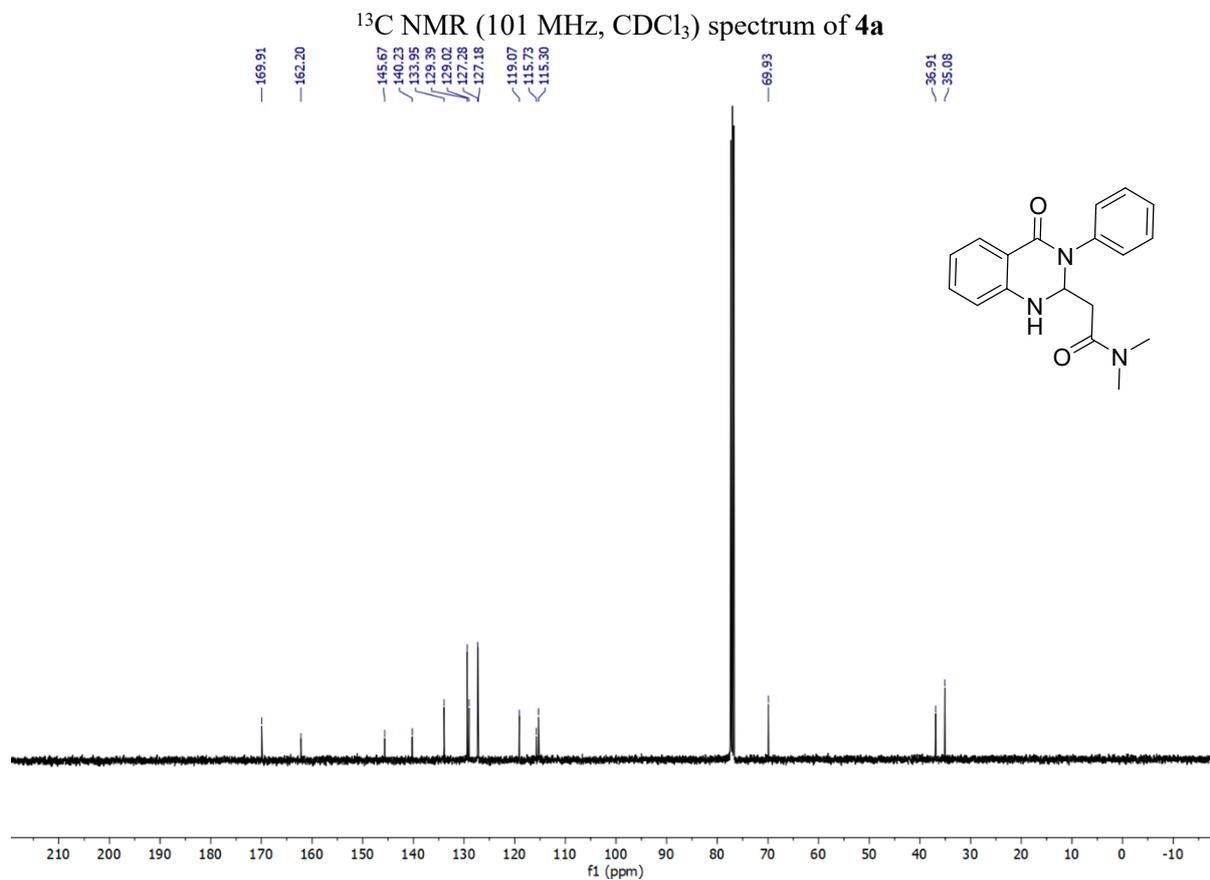
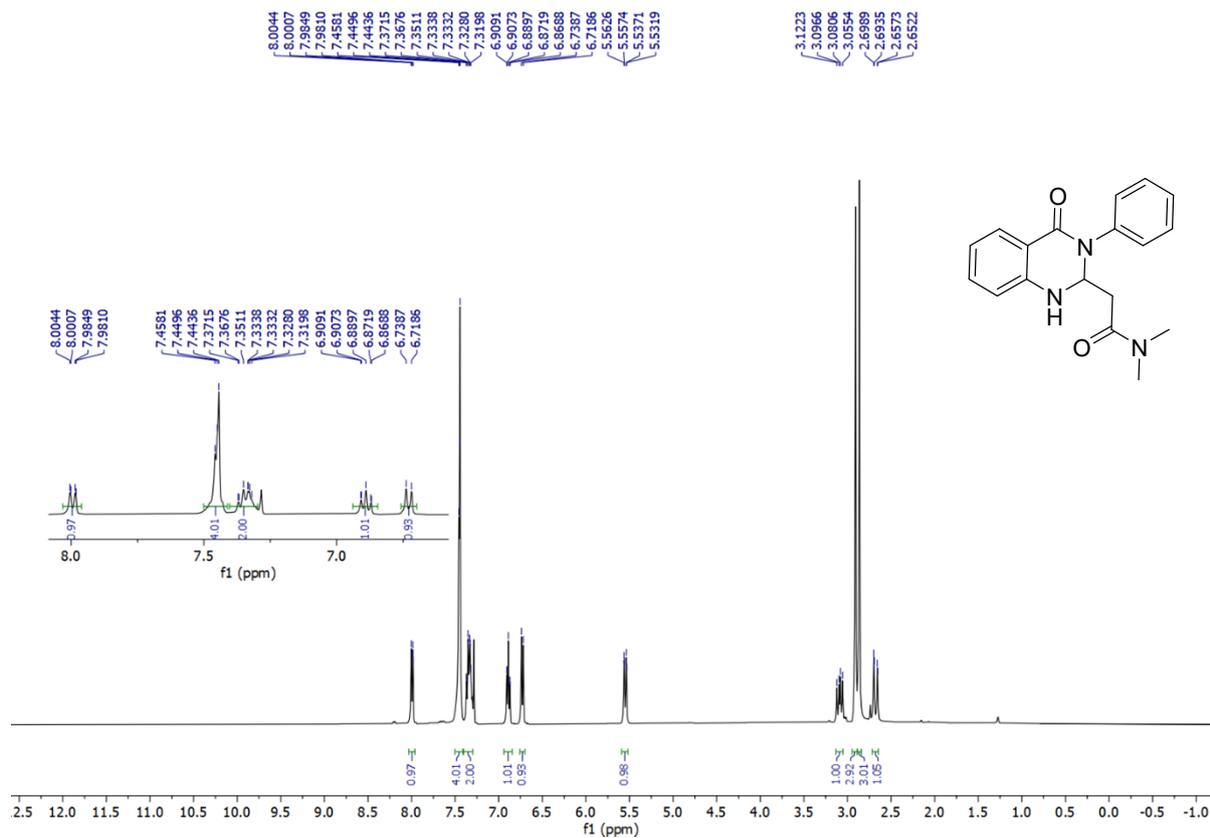
N-(tert-butyl)-2-(4-oxo-3-phenyl-1,2,3,4-tetrahydroquinazolin-2-yl) acetamide (4j)



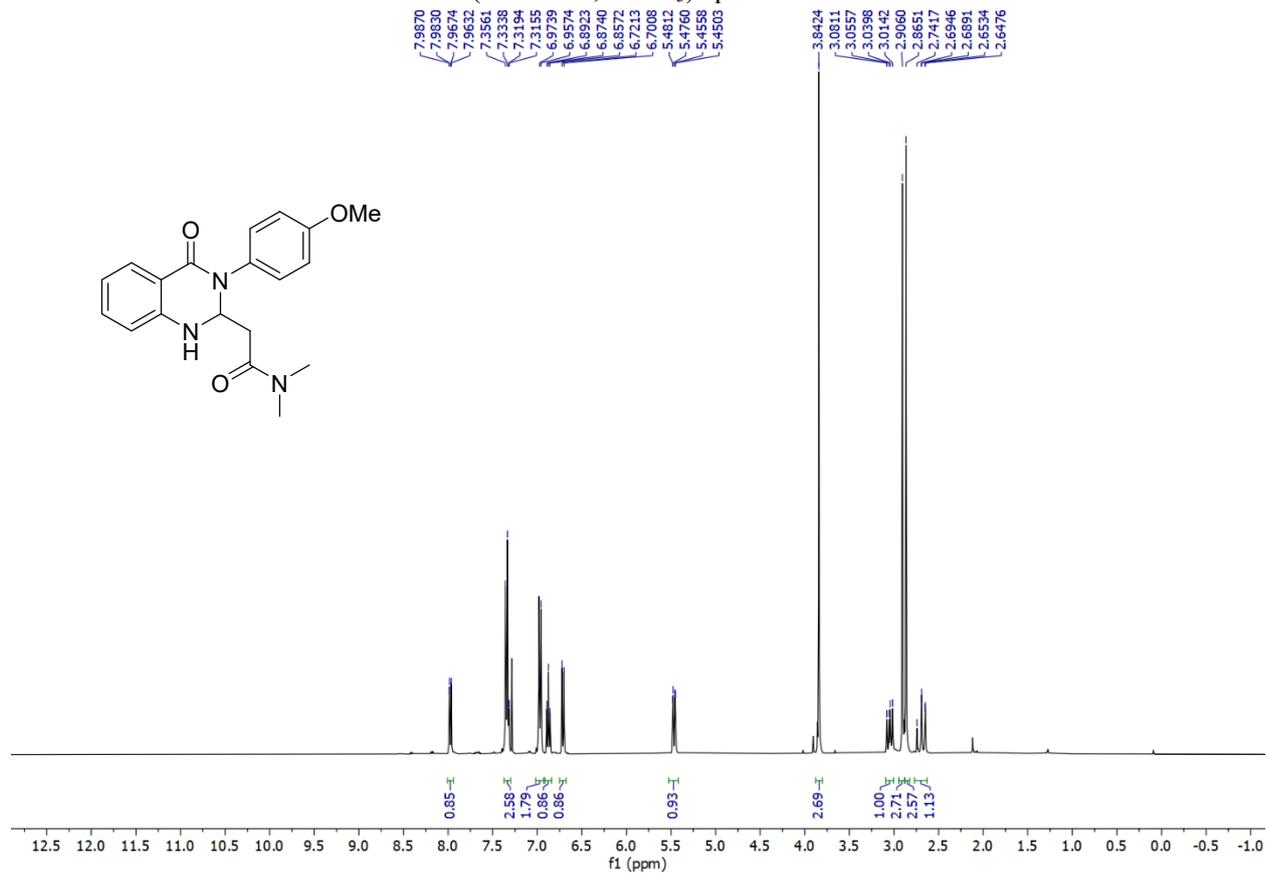
Cream solid (13.4 mg, yield 40%); mp 202-205 °C; 1H NMR (499 MHz, $CDCl_3$) δ_H 7.95 (d, $J = 7.8$ Hz, 1H), 7.42 (t, $J = 7.6$ Hz, 2H), 7.36 (d, $J = 8.1$ Hz, 2H), 7.33 (d, $J = 7.4$ Hz, 1H), 7.31 (s, 1H), 7.25 (s, 1H), 6.88 (t, $J = 7.5$ Hz, 1H), 6.75 (d, $J = 8.1$ Hz, 1H), 5.47 – 5.41 (m, 1H), 5.33 (s, 1H), 2.88 (dd, $J = 15.5, 10.3$ Hz, 1H), 2.49 (dd, $J = 15.6, 2.5$ Hz, 1H), 1.29 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.2, 165.7, 145.7, 140.1, 134.0, 133.1, 129.6, 129.4, 127.5, 127.3, 119.9, 115.4, 69.8, 51.7, 38.3, 29.0, 28.9, 28.7. Anal. Calcd for $C_{20}H_{23}N_3O_2$: C, 71.19; H, 6.87; N, 12.45; Found: C, 71.50; H, 7.05; N, 12.71.

5. Copies of 1H and ^{13}C NMR spectra of products

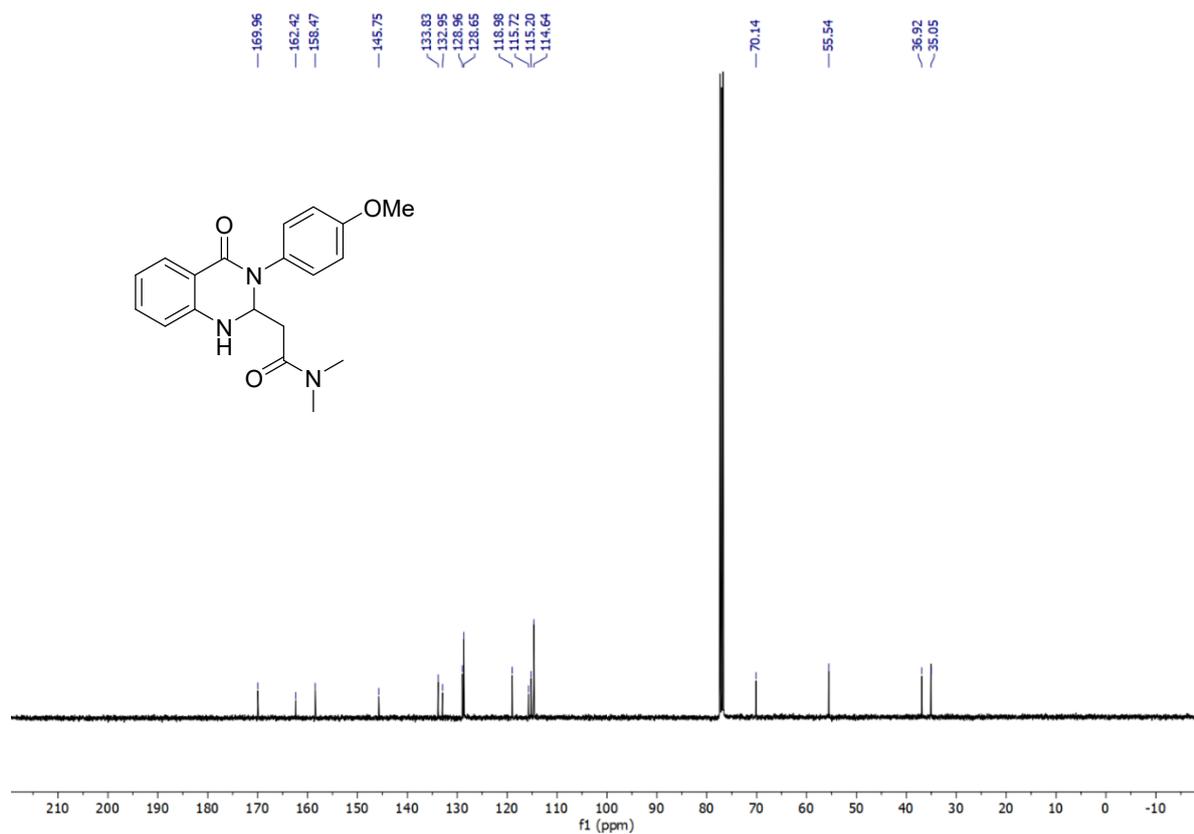
1H NMR (400 MHz, $CDCl_3$) spectrum of **4a**



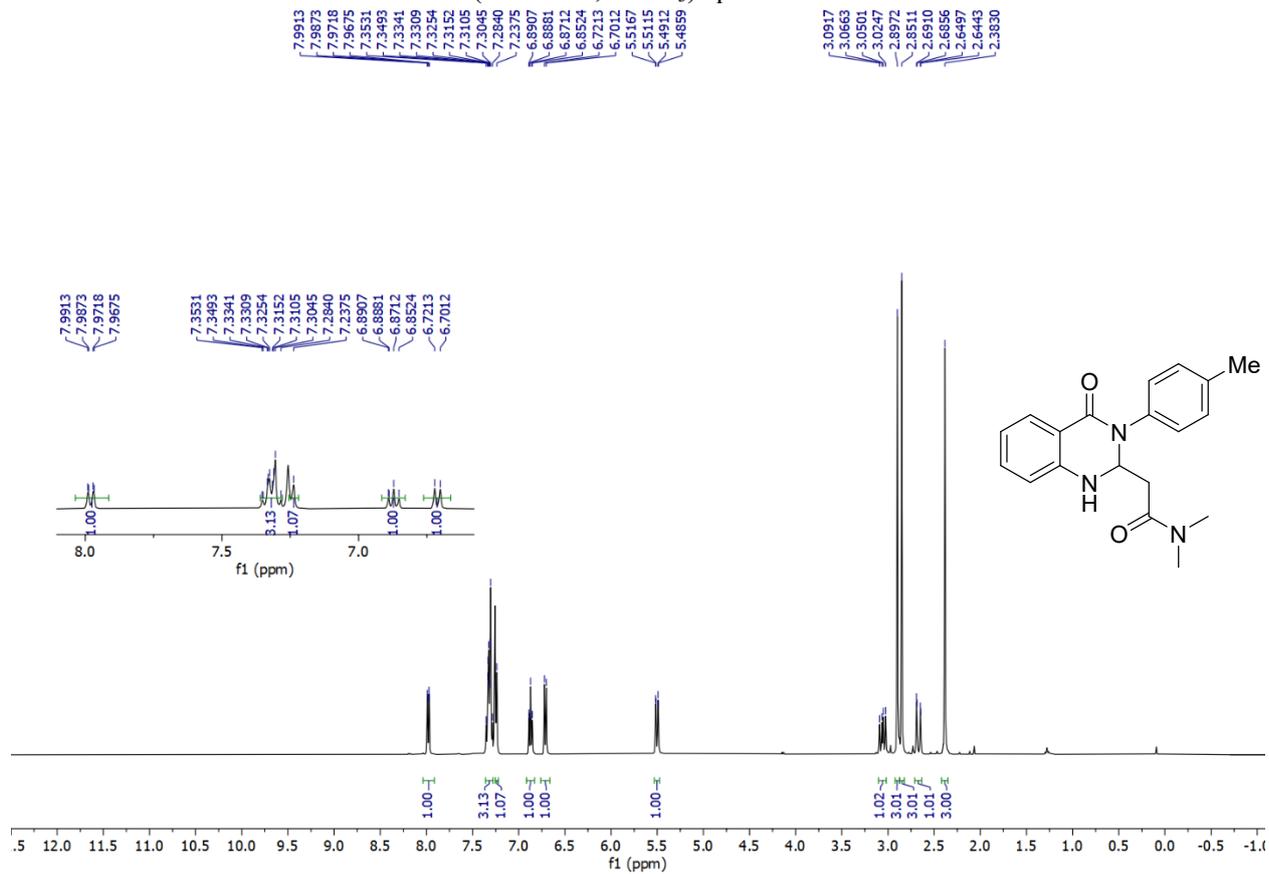
¹H NMR (400 MHz, CDCl₃) spectrum of **4b**



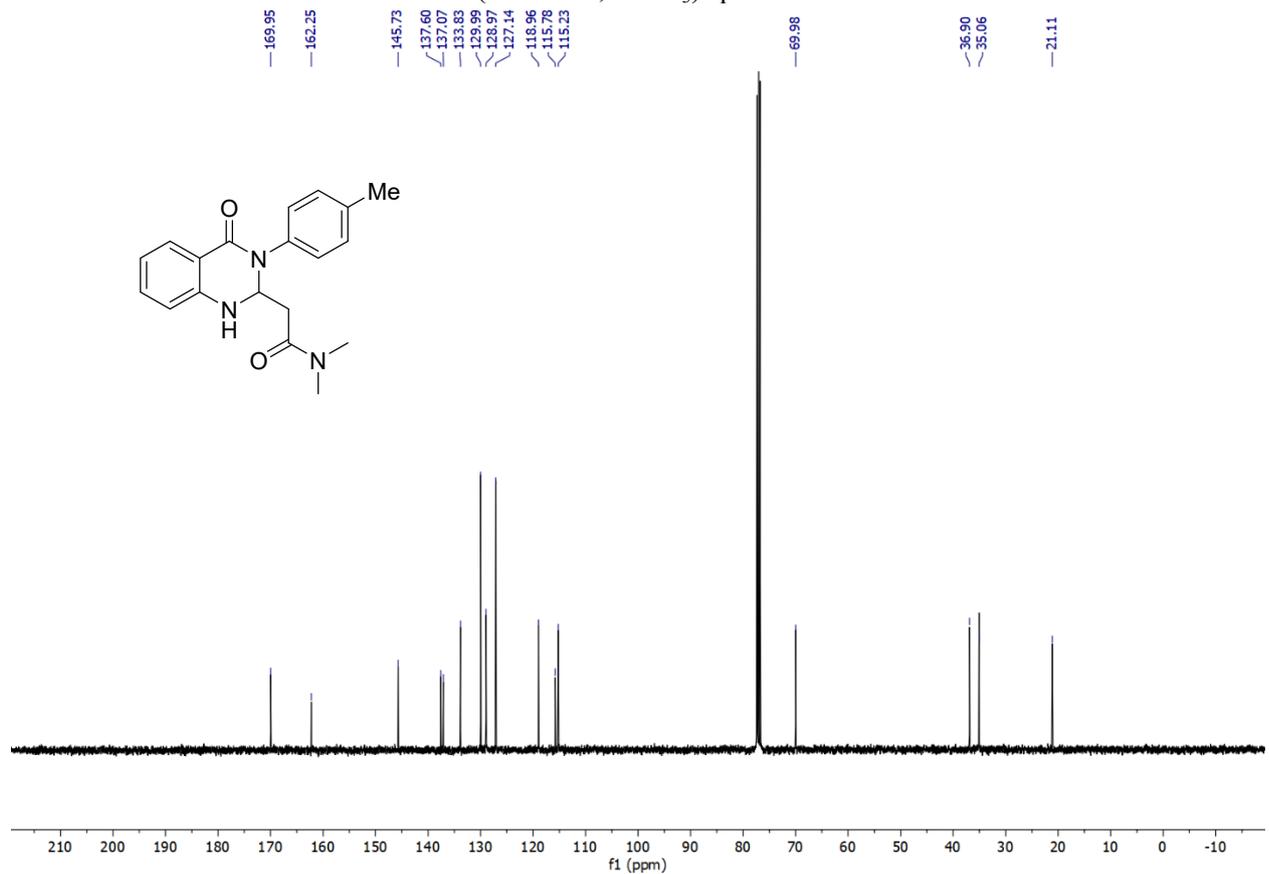
¹³C NMR (101 MHz, CDCl₃) spectrum of **4b**

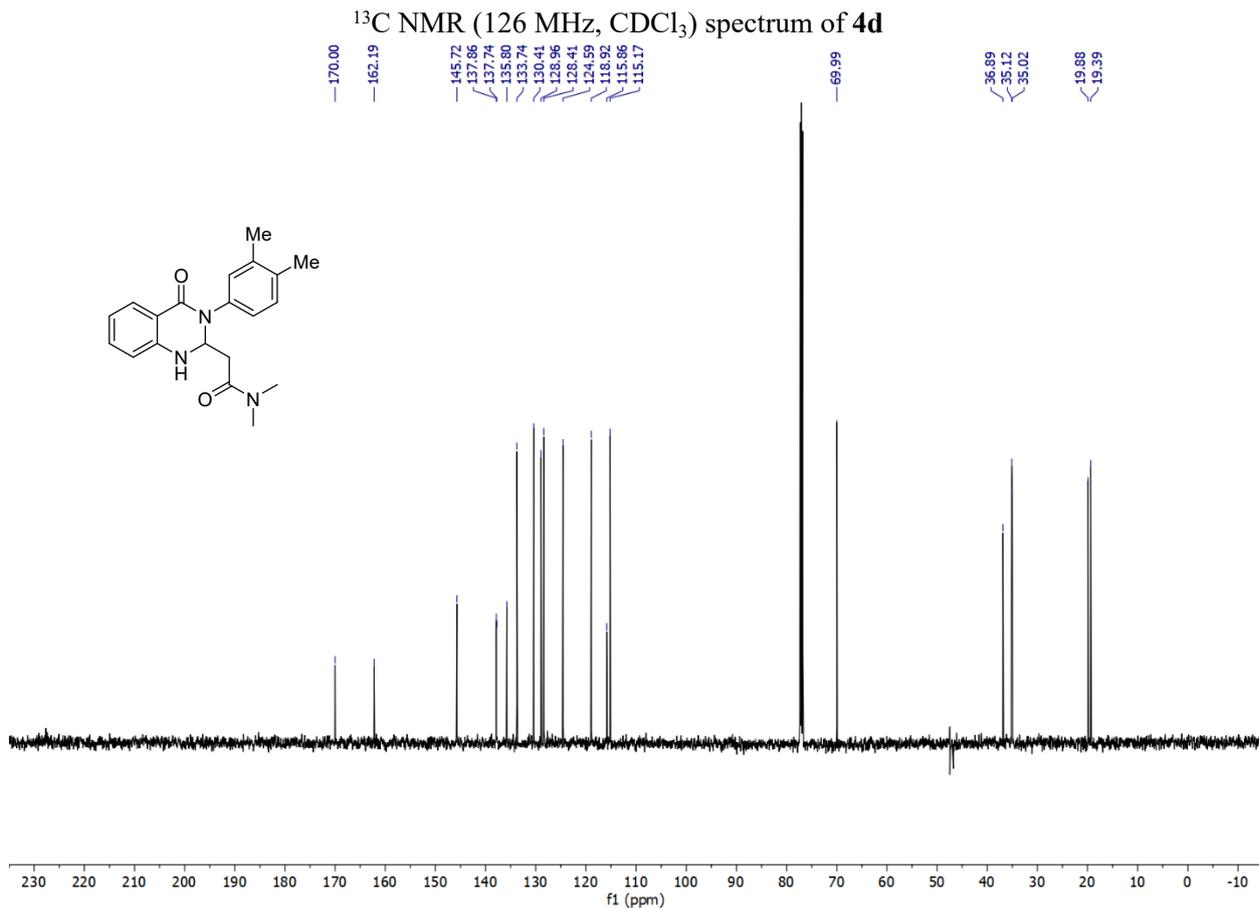
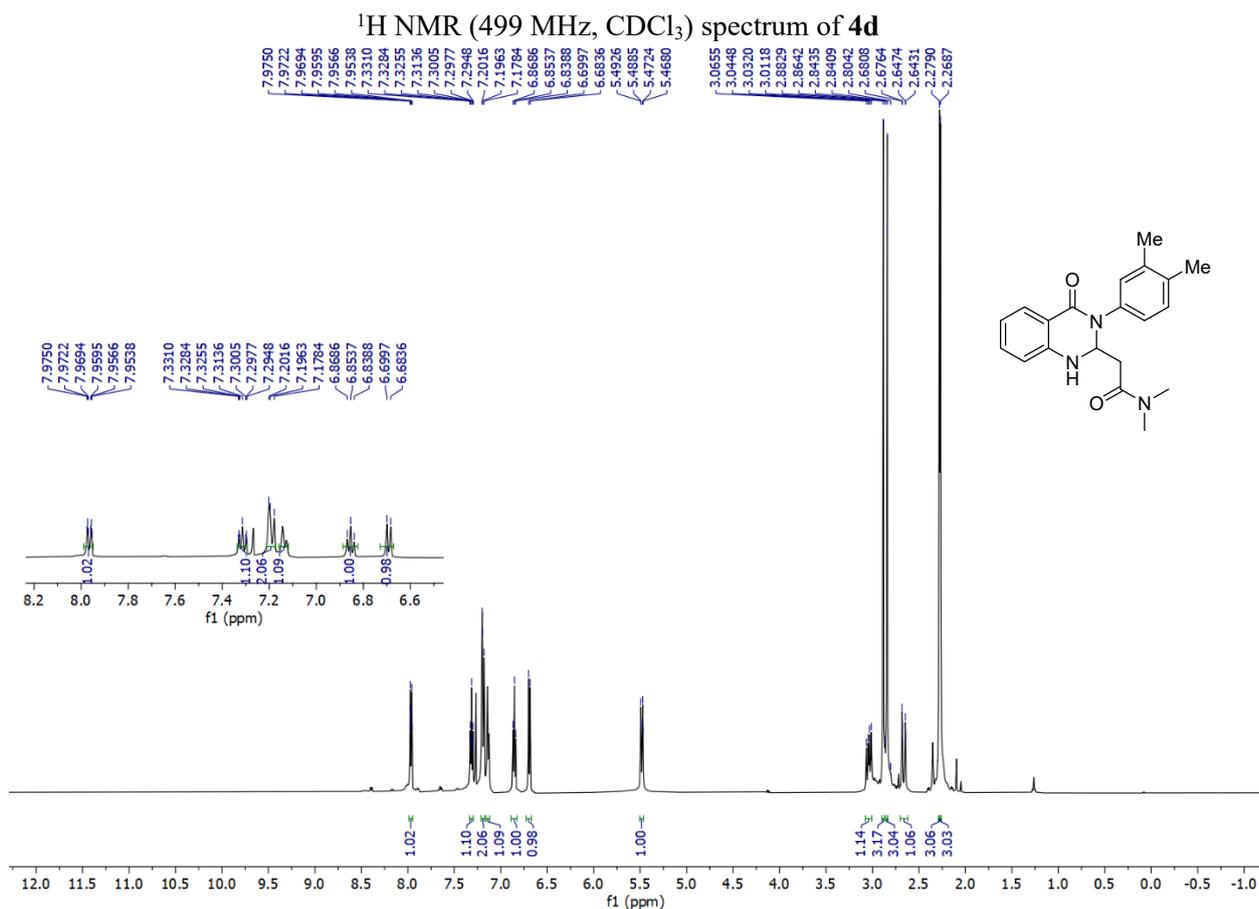


¹H NMR (400 MHz, CDCl₃) spectrum of **4c**

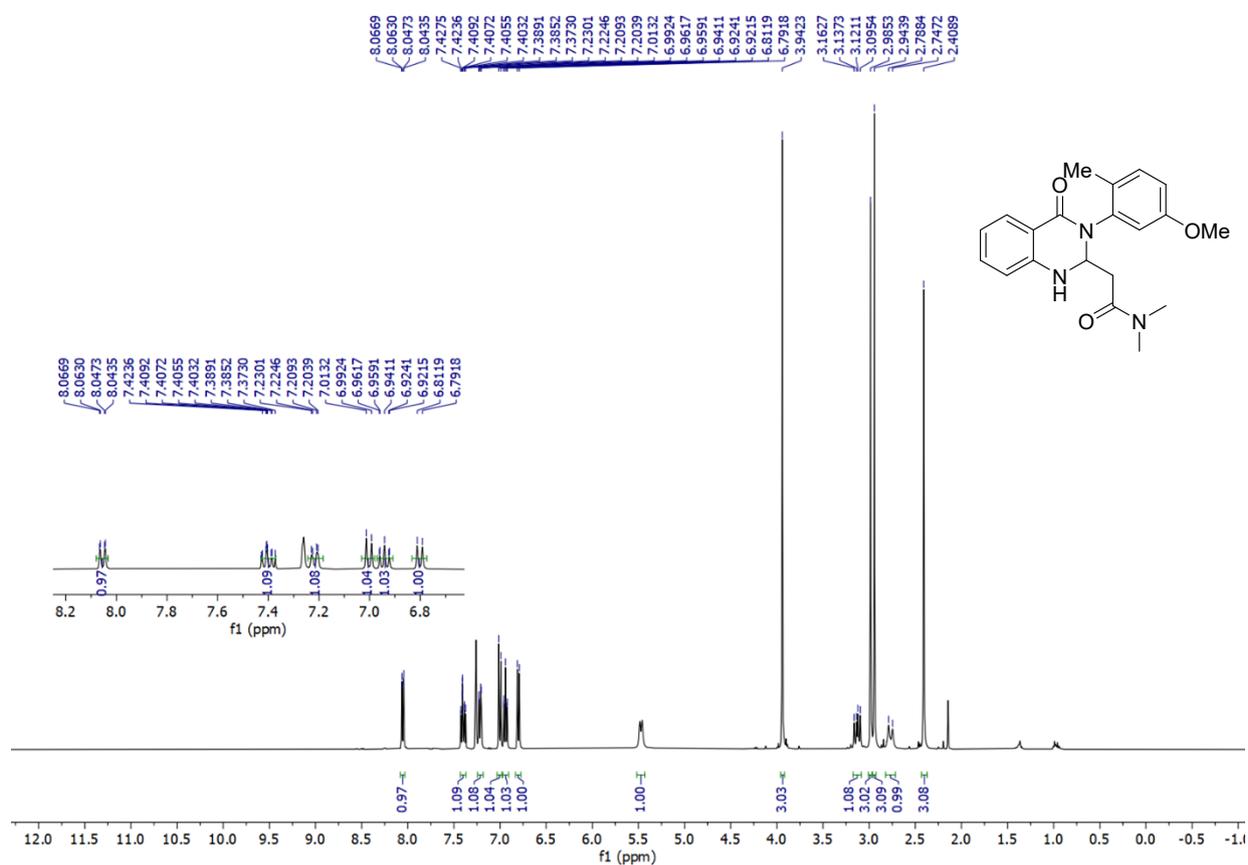


¹³C NMR (101 MHz, CDCl₃) spectrum of **4c**

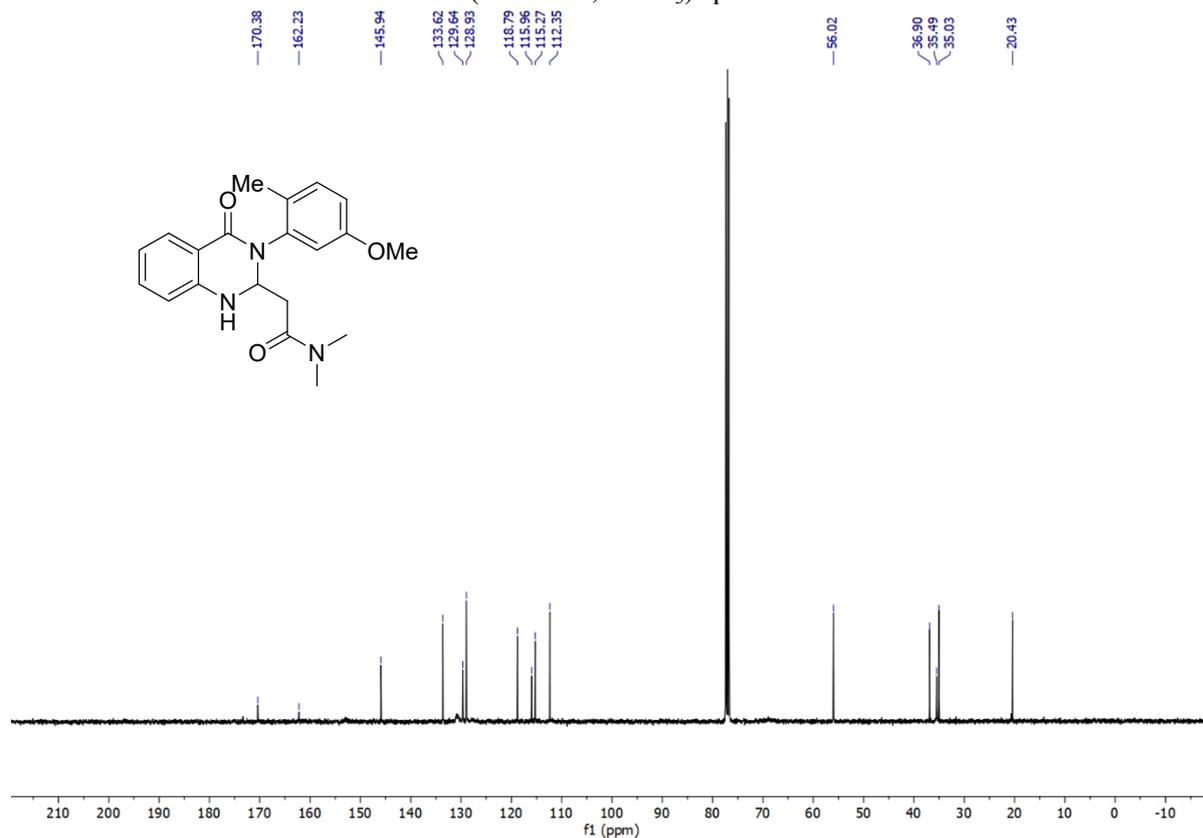




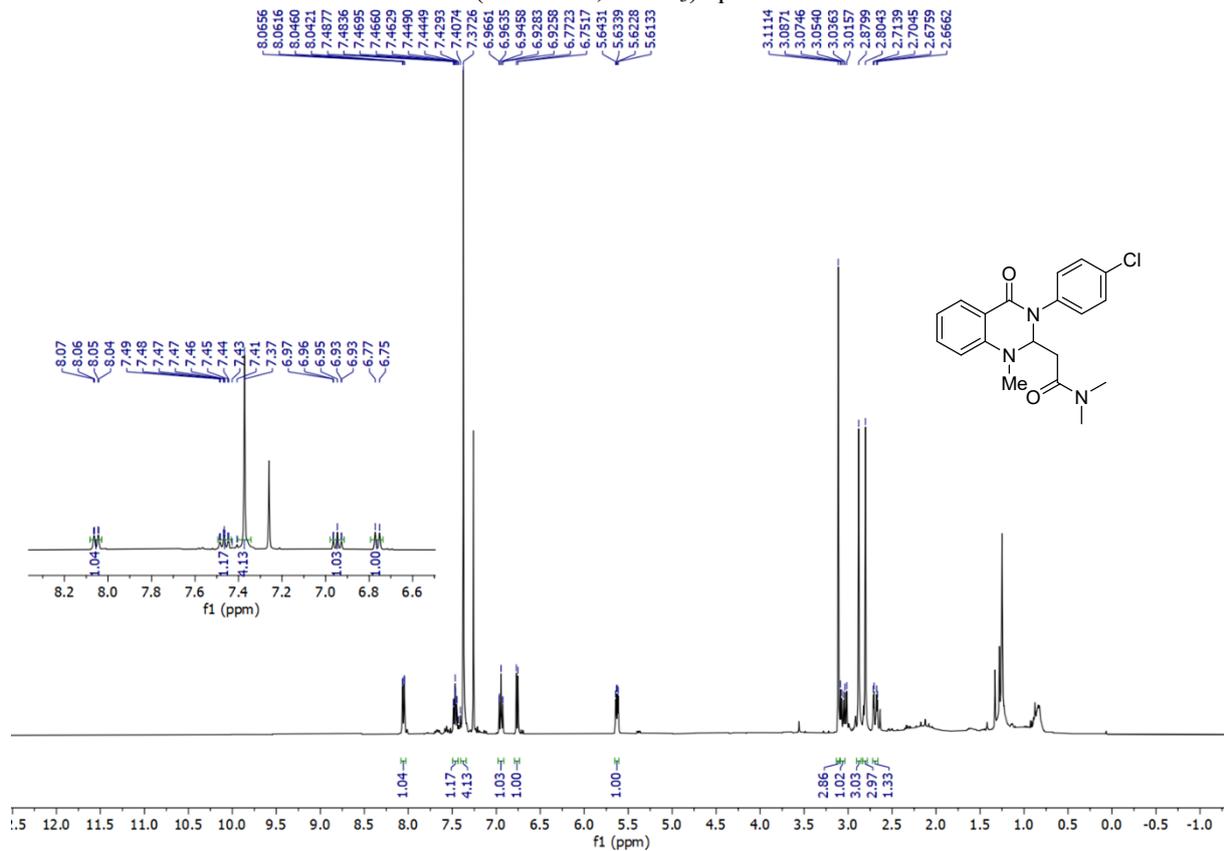
¹H NMR (400 MHz, CDCl₃) spectrum of **4e**



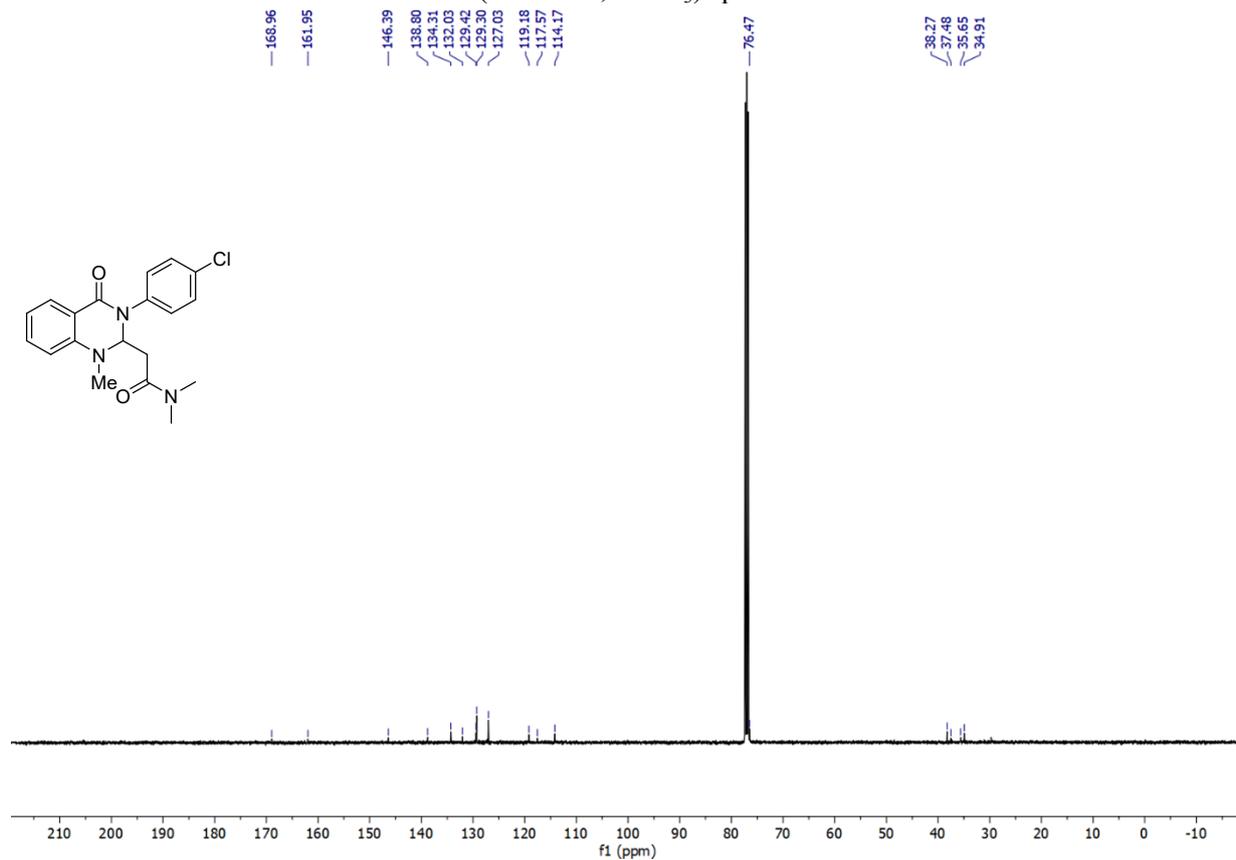
¹³C NMR (101 MHz, CDCl₃) spectrum of **4e**



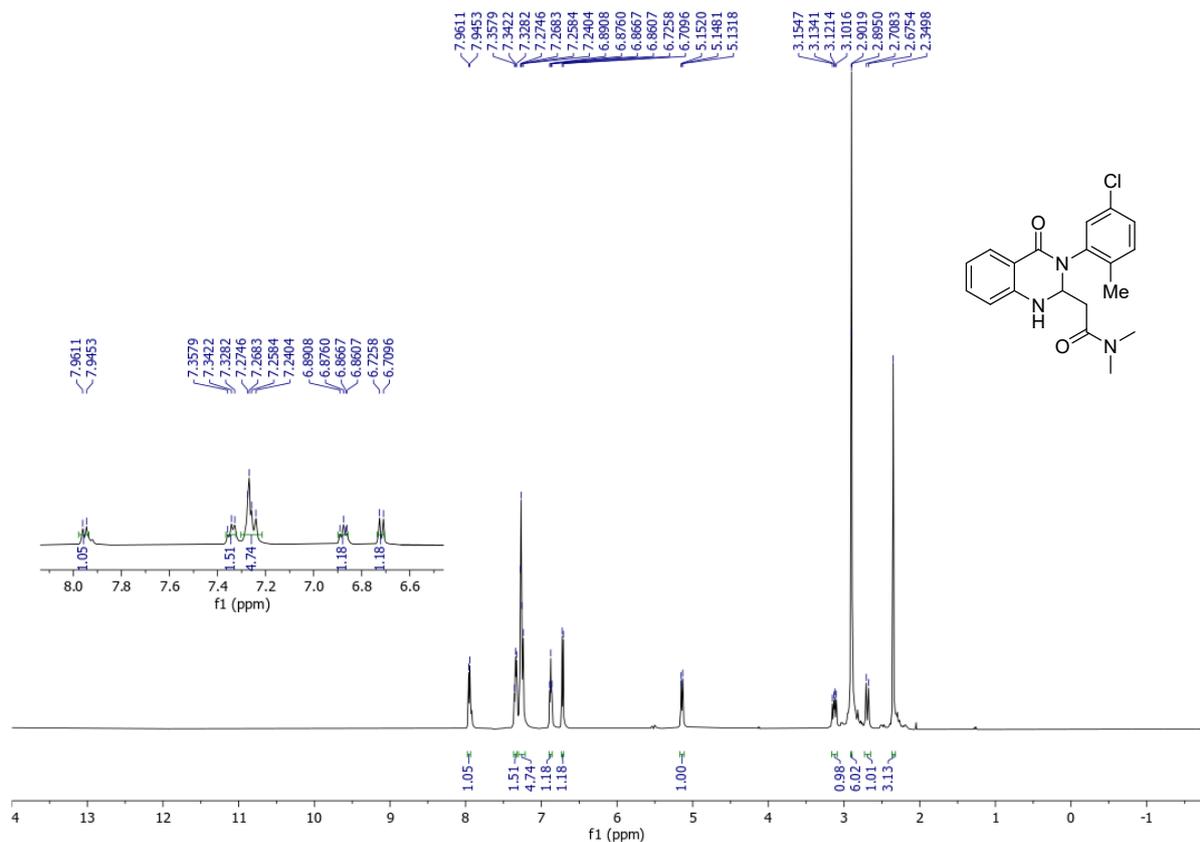
¹H NMR (400 MHz, CDCl₃) spectrum of **4f**



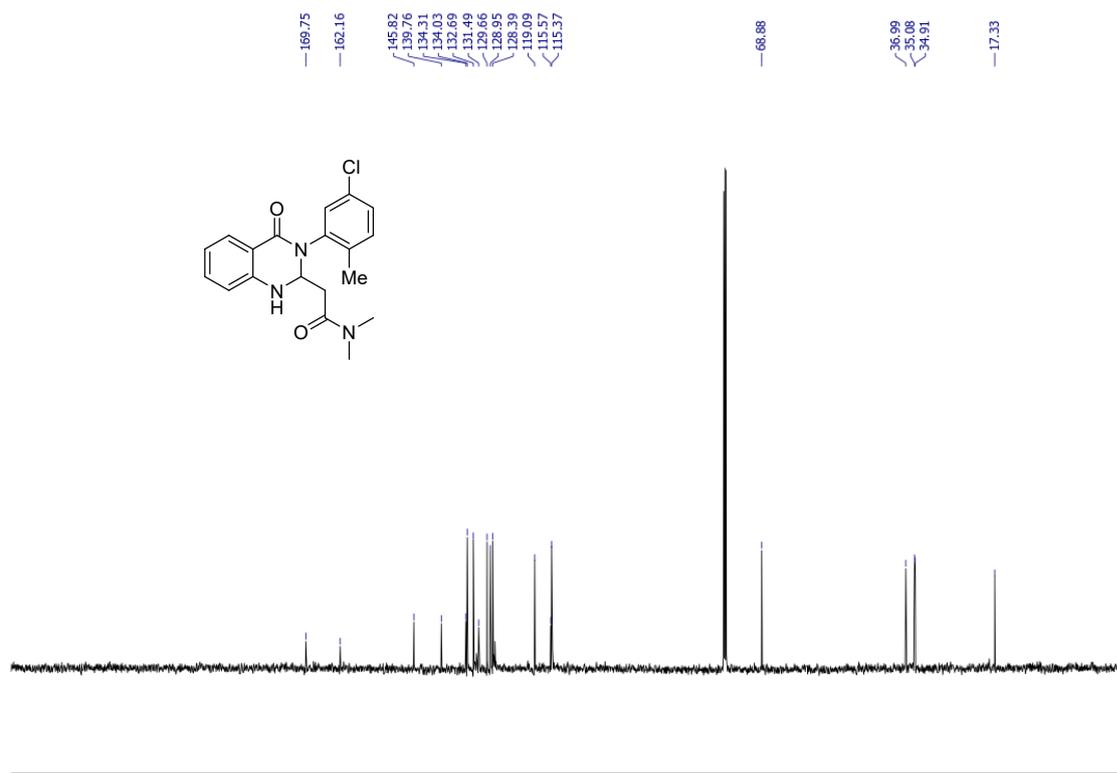
¹³C NMR (101 MHz, CDCl₃) spectrum of **4f**



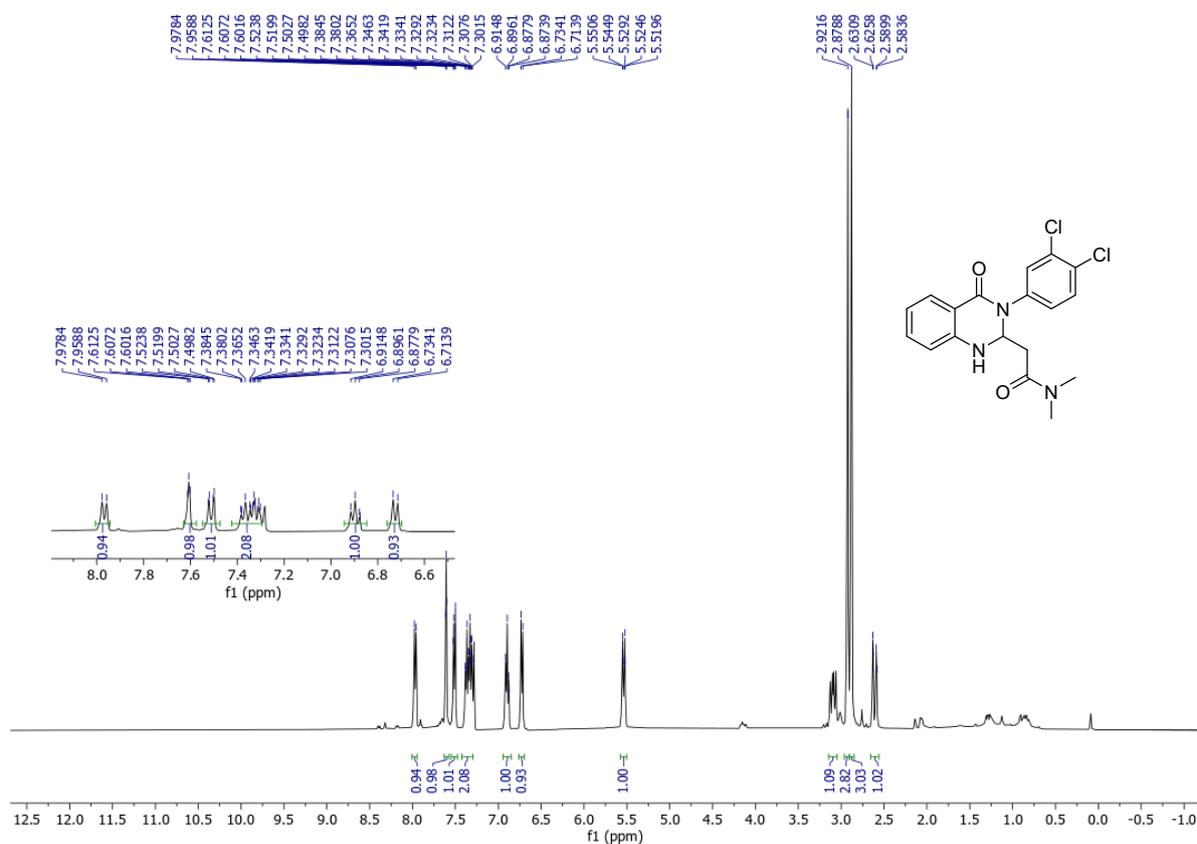
¹H NMR (499 MHz, CDCl₃) spectrum of **4g**



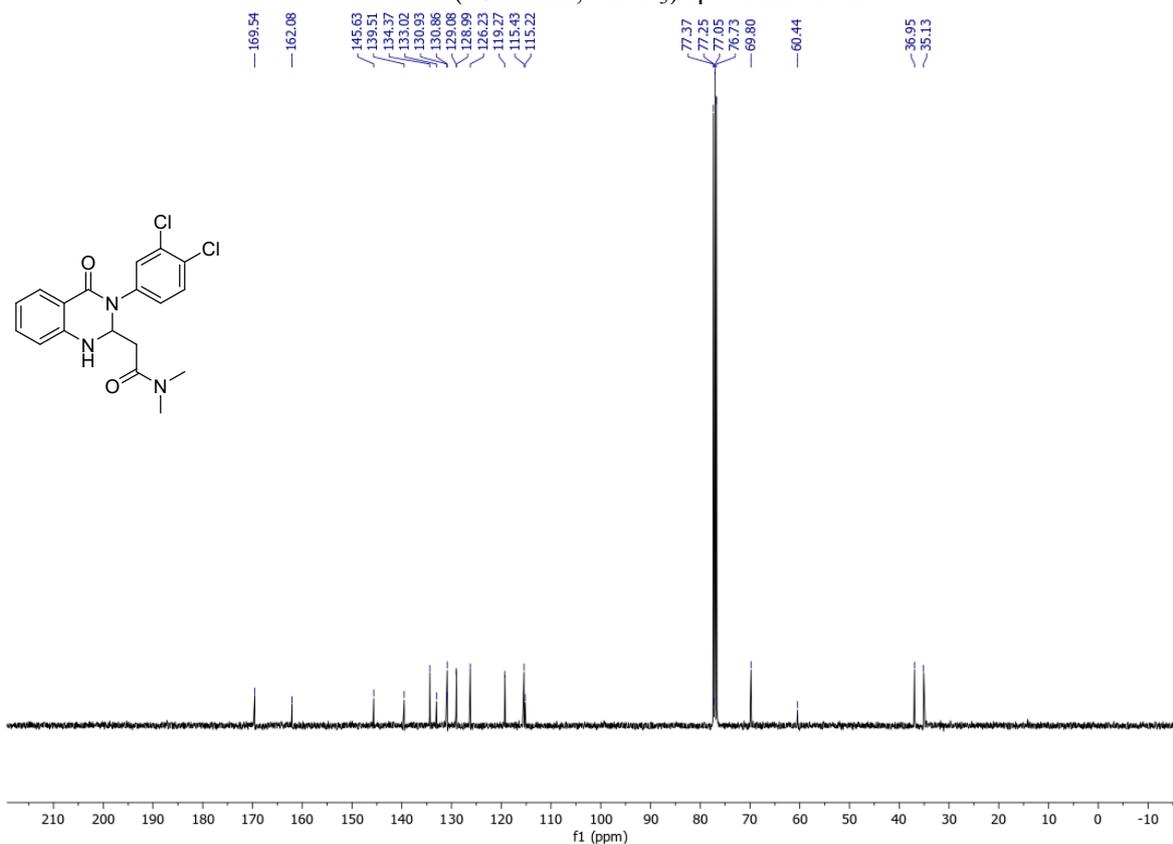
¹³C NMR (126 MHz, CDCl₃) spectrum of **4g**



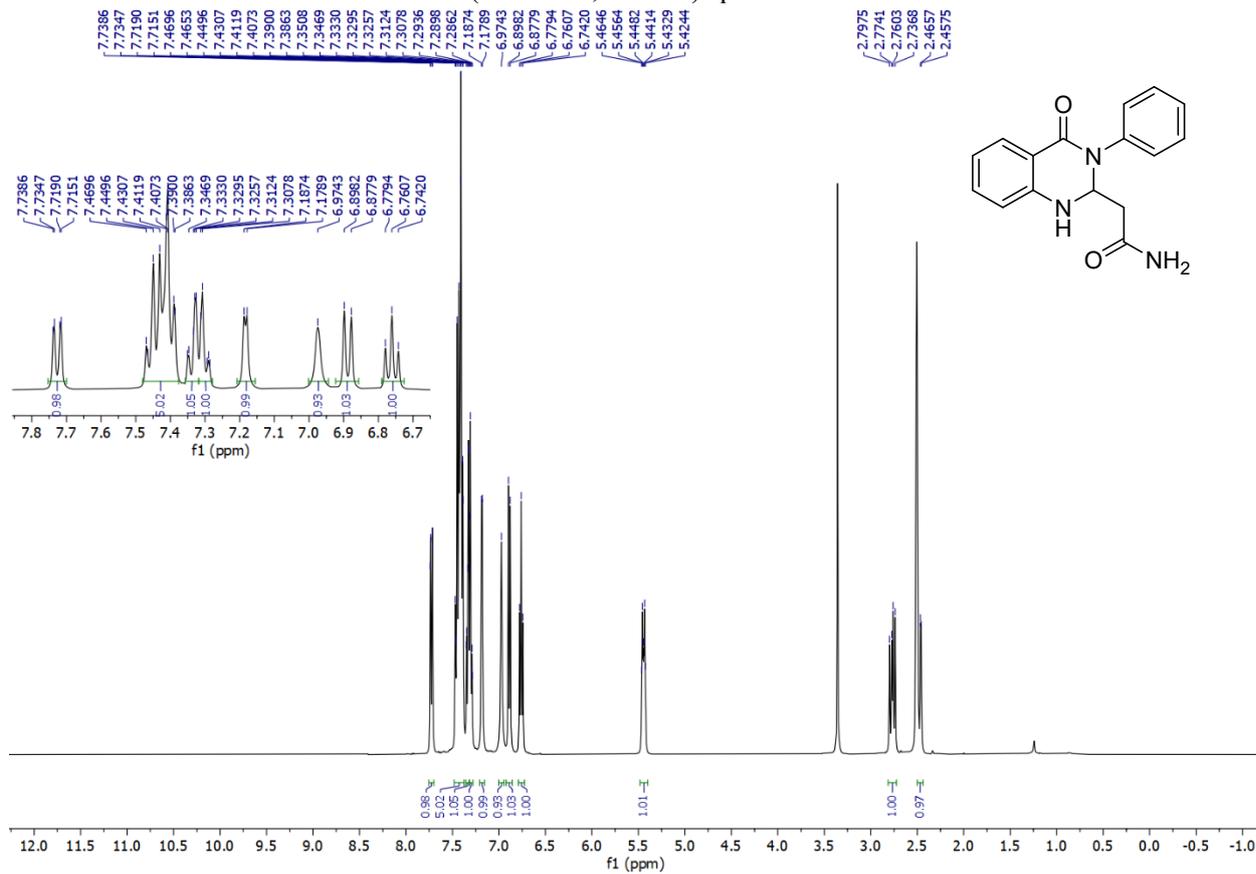
¹H NMR (400 MHz, CDCl₃) spectrum of **4h**



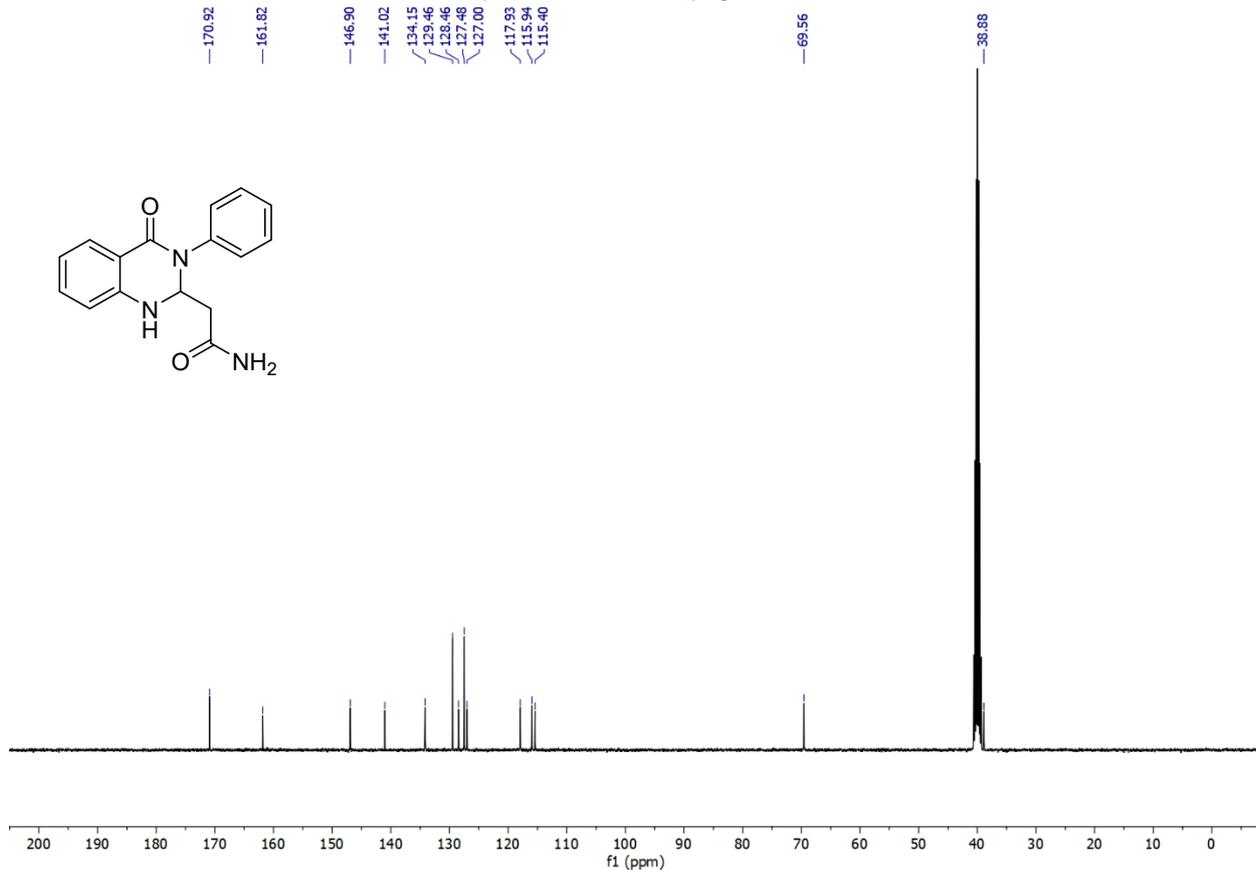
¹³C NMR (101 MHz, CDCl₃) spectrum of **4h**



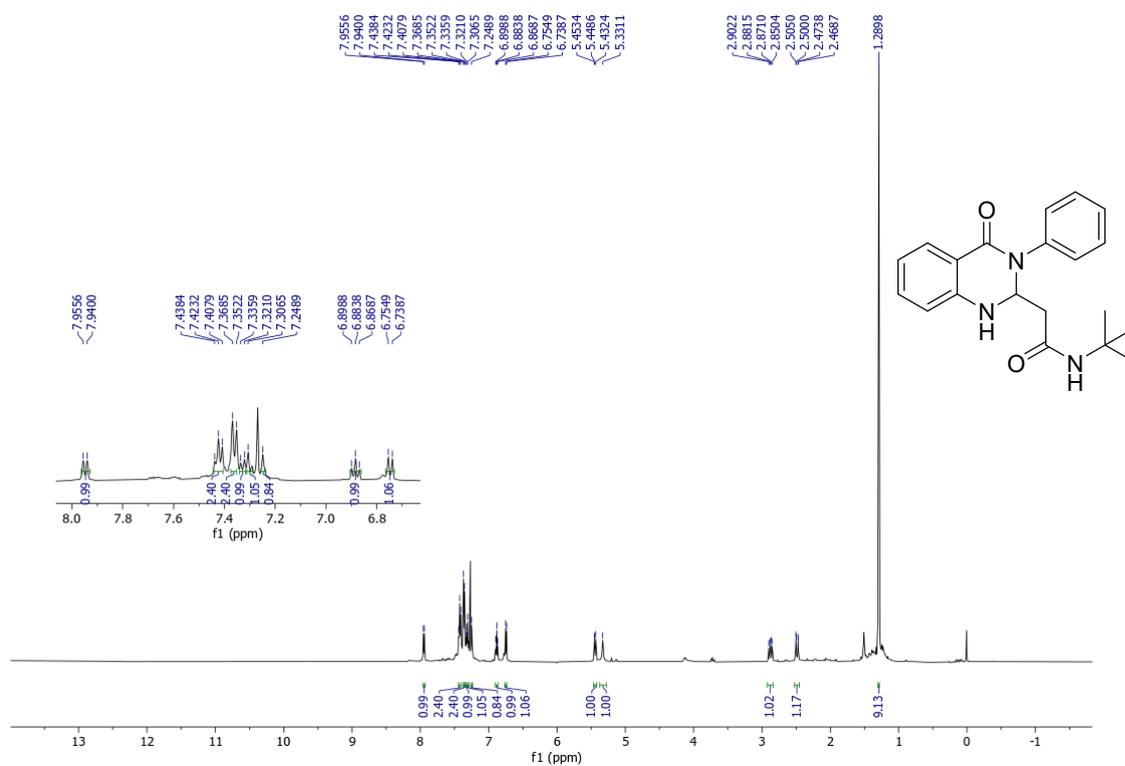
¹H NMR (400 MHz, DMSO) spectrum of **4i**



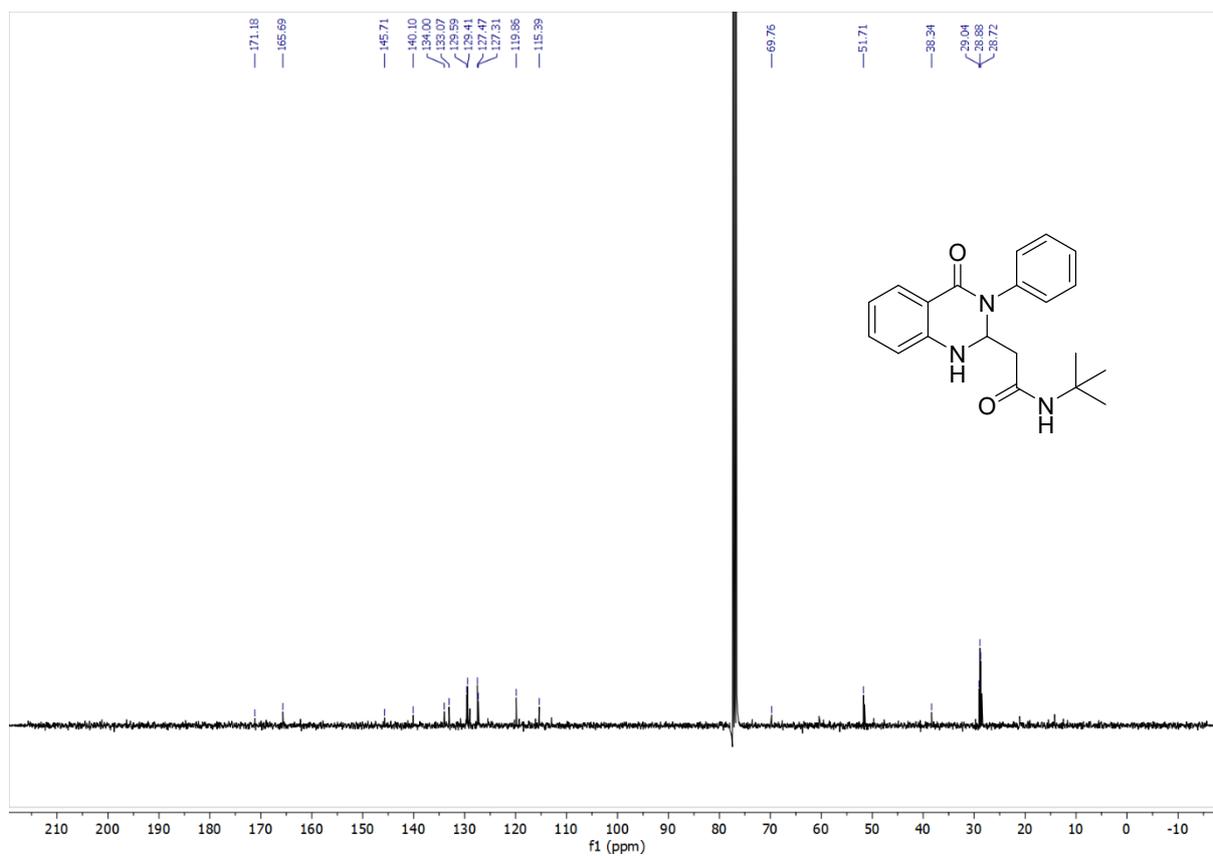
¹³C NMR (101 MHz, CDCl₃) spectrum of **4i**



¹H NMR (499 MHz, CDCl₃) spectrum of **4j**



¹³C NMR (126 MHz, CDCl₃) spectrum of **4j**



6. Computational details

All reported structures were fully optimized using Gaussian 16¹ at the M06-L level of theory.² This functional has been widely validated and is known to provide accurate results for transformations involving transition metal complexes.³ Solvent effects were accounted for using the SMD solvation model⁴ with water as the solvent, and Grimme's GD3 empirical dispersion corrections were included in all calculations. Geometry optimizations employed the SDD basis set with effective core potential (ECP) for Au and I atoms, while 6-31G(d) was used for all other atoms.⁵; this combination is referred to as BS1. Frequency analyses were conducted at the same level of theory to confirm the nature of stationary points. Transition states were located using the Berny algorithm, and their connectivity to reactants and products was verified by intrinsic reaction coordinate (IRC) calculations.⁶ To improve the accuracy of computed energies, single-point calculations were performed using the M06-L-D3 functional with a larger basis set, BS2, which consists of SDD (with ECP) for Au and I and 6-311+G(2d,p) for all other atoms.

The overall solvation free energies were obtained by combining the thermal corrections from frequency calculations with the single-point solvation energies from the SMD model. Additionally, a standard-state correction of $\Delta G^{\text{atm} \rightarrow 1\text{M}} = 1.89$ kcal/mol was applied to account for compressing 1 mol of an ideal gas from 1 atm to the 1 M solution phase.

Mechanism of anthranilamide formation from isatoic anhydride and aniline. The reaction between isatoic anhydride **1a** and aniline **2a** proceeds via nucleophilic attack of aniline at the C1 carbonyl carbon of isatoic anhydride, leading to heterolytic cleavage of the C1–O1 σ bond and formation of a zwitterionic intermediate **5A**. This step occurs through transition structure **TS_{1a-5A}** (Figure S2) with a computed free-energy barrier of 27.1 kcal/mol and is the rate-determining step of the pre-catalytic anthranilamide-forming process.

The zwitterionic nature of intermediate **5A** suggests that this species is better stabilised through hydrogen-bonding interactions with the solvent, which in this case is water. To account for this effect, we included two explicit water molecules as a minimal solvent cluster in the calculations. These hydrogen-bonding interactions lead to formation of intermediate **5B** and result in an additional stabilisation of the system by 7.5 kcal/mol.

In addition to stabilising the zwitterionic intermediate **5A**, the explicit water cluster can also act as a proton shuttle. This enables proton transfer from the ammonium group to the carboxylate moiety in intermediate **5B** via transition structure **TS_{5B-5C}**, leading to formation of the more stable intermediate **5C**. All attempts to identify an (H₂O)₂-mediated proton transfer from the ammonium group to the N1 atom in **5B** were unsuccessful, as proton transfer consistently occurred to the carboxylate group instead. Finally, proton transfer from the carboxylic acid group to the N1 atom in **5D** results in formation of anthranilamide **5**.

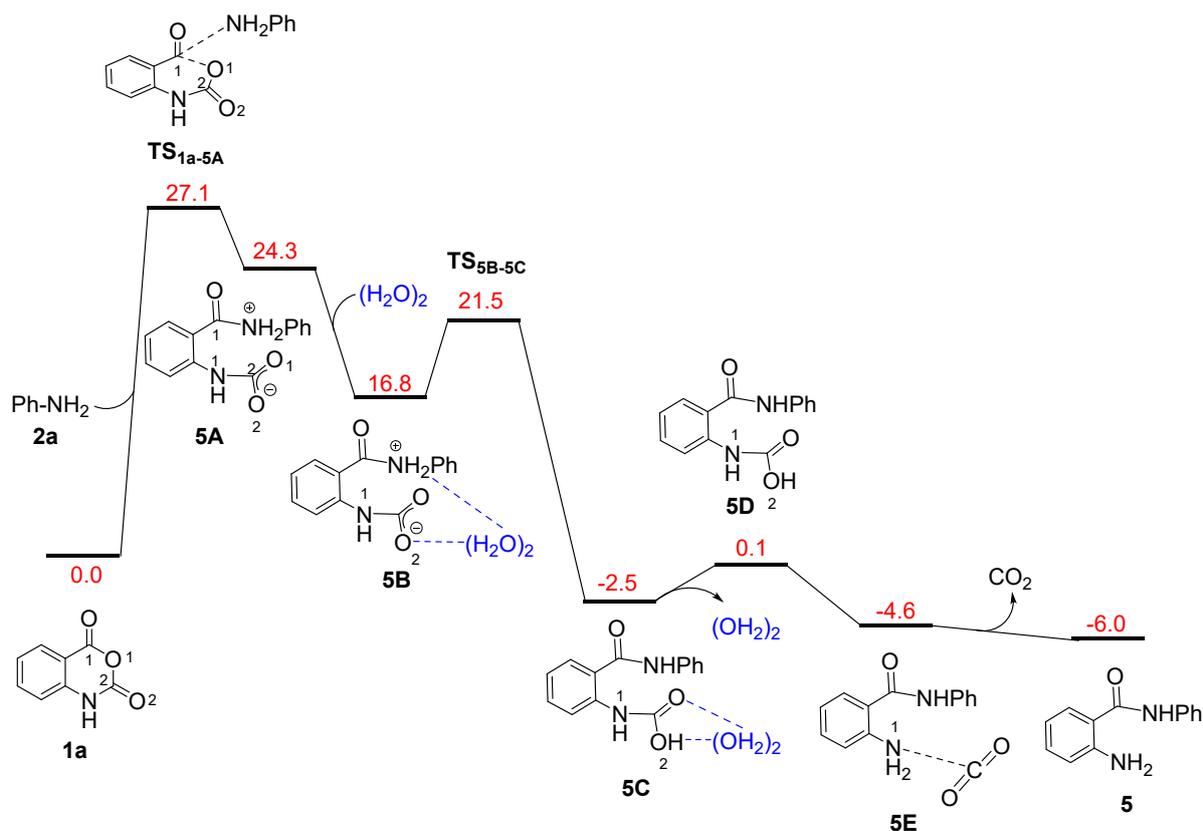


Fig. S2 Computed free-energy profile for the reaction of isatoic anhydride **1a** with aniline **2a** leading to anthranilamide **5**. Relative free energies were calculated at the SMD/M06-L-D3/SDD,6-311+G(2d,p)//SMD/M06-L-D3/SDD,6-31G(d) level of theory in water and are reported in kcal/mol.

Solvent effects on the formation of anthranilamide 5. To understand why the reaction exhibits the highest reactivity in water, we examined computationally the mechanism for formation of anthranilamide **5** from isatoic anhydride **1a** and aniline **2a**, as this step has the largest activation free energy in the computed mechanism. Solvent effects on this step were then analysed by performing additional calculations in two representative aprotic solvents, acetonitrile and toluene (Figure S3). Experimentally, only a low yield was obtained in acetonitrile (24%), whereas no desired product was observed in toluene (Table 1).

The calculations indicate that the mechanism for forming **5** in these aprotic solvents differs from that in protic water. In acetonitrile and toluene, aniline nucleophilic attack (N–C1 bond formation) and deprotonation of N–H1 by O1 occur concertedly through a single transition structure (TS_{1a-5D}), leading directly to intermediate **5D**. Importantly, the computed activation barriers in these aprotic solvents are substantially higher than in water (27.1 kcal/mol in water, 32.5 kcal/mol in acetonitrile, and 34.5 kcal/mol in toluene). This increase is consistent with the zwitterionic character of the transition structure associated with aniline attack at C1 of **1a**, which is better stabilised in protic media. The higher barrier in toluene relative to acetonitrile can be attributed to the much lower dielectric constant of toluene ($\epsilon = 2.37$) compared to acetonitrile ($\epsilon = 35.68$), which provides poorer stabilisation of a transition structure with zwitterionic character and therefore increases the activation barrier.

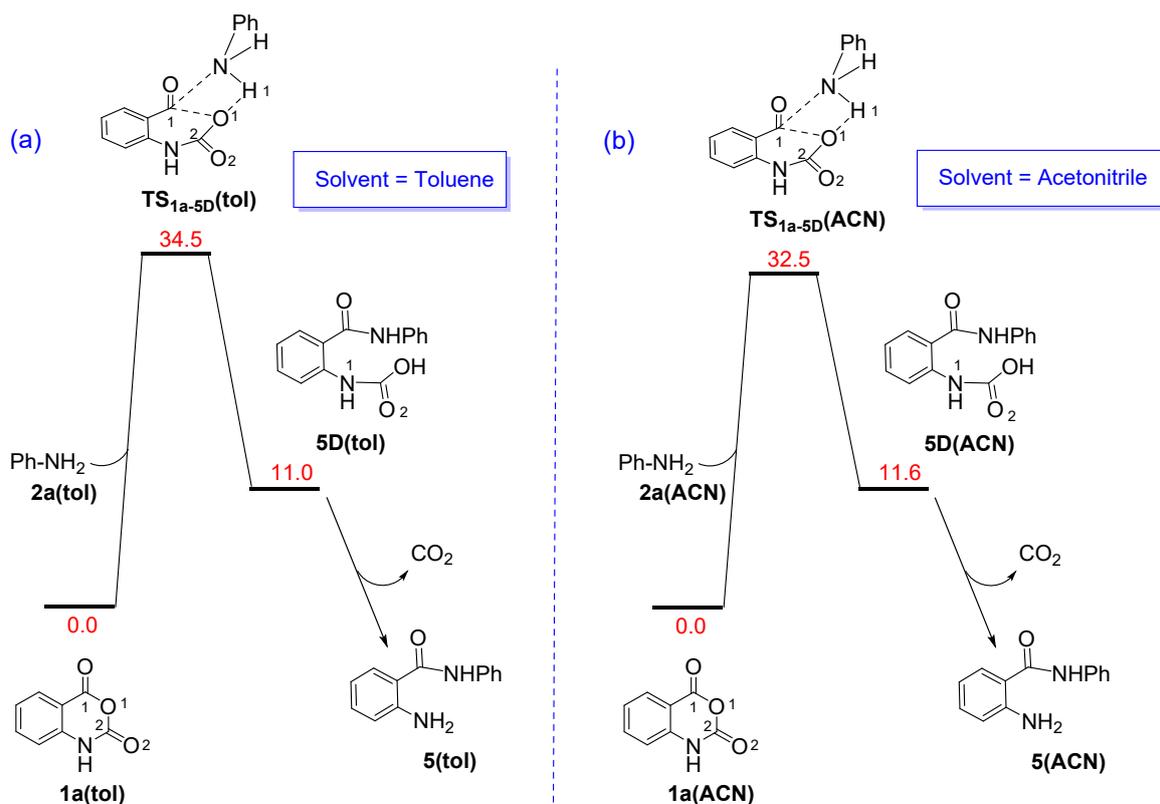


Figure S3. Computed free-energy profiles for the formation of anthranilamide **5** from isatoic anhydride **1a** and aniline **2a** in (a) toluene and (b) acetonitrile. Relative free energies were calculated at the SMD/M06-L-D3/SDD,6-311+G(2d,p)//SMD/M06-L-D3/SDD,6-31G(d) level of theory and are reported in kcal/mol.

Substituent effects on the formation of anthranilamide 5: To analyse substituent effects in more detail, we focused on the step that we computationally identified as the rate-determining step of the reaction, namely the nucleophilic attack of aniline **2** on isatoic anhydride **1a** leading to intermediate **5**. We examined the effect of substituents on the aniline ring by computing activation barriers for X = OMe, H, and NO₂ (Figure S4).

The calculated activation barriers follow the trend $\Delta G^\ddagger = 24.2$ kcal/mol (X = OMe) < 27.1 kcal/mol (X = H) << 37.4 kcal/mol (X = NO₂), which is in excellent agreement with the experimental observations. Experimentally, reactions with X = H or OMe proceed smoothly and afford the desired products in good yields, whereas no product formation is observed for X = NO₂.

These results show that the reactivity is primarily controlled by the nucleophilicity of the aniline, which is strongly influenced by the electronic nature of the substituent. The strongly electron-withdrawing NO₂ group significantly reduces the nucleophilicity of aniline, leading to a prohibitively high activation barrier and rendering formation of intermediate **5** kinetically inaccessible. In contrast, electron-neutral or electron-donating substituents (H and OMe) maintain sufficient nucleophilicity to allow the reaction to proceed.

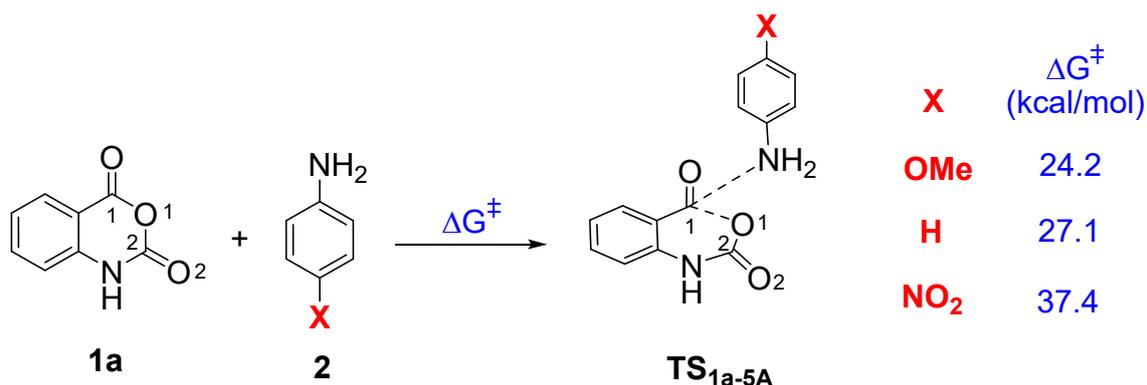


Figure S4. Computed activation free energies (ΔG^\ddagger , kcal/mol) for nucleophilic attack of substituted anilines ($X = \text{OMe}, \text{H}, \text{NO}_2$) on isatoic anhydride **1a** leading to **TS_{1a-5A}**. Relative free energies were calculated at the SMD/M06-L-D3/SDD,6-311+G(2d,p)//SMD/M06-L-D3/SDD,6-31G(d) level of theory and are reported in kcal/mol.

Formation of the Pd(II)–hydroperoxo species: hydrogen-atom abstraction by O₂. A well-established and widely accepted mechanism for formation of Pd(II)–hydroperoxo species involves reaction of triplet O₂ with a Pd(II)–H intermediate via a hydrogen-atom abstraction pathway. In this mechanism, triplet O₂ acts as a hydrogen-radical abstractor from the Pd–H bond, generating a Pd(I) species together with an HO₂[•] radical. Subsequent recombination of the HO₂[•] radical with Pd(I) affords a triplet hydroperoxo–Pd complex, which then undergoes efficient intersystem crossing to the singlet surface to give the Pd(II)–hydroperoxo species. This pathway has been extensively discussed and supported by numerous previous computational studies (see refs 27 and 36-42)

In Figure S5, we have explicitly computed this mechanism. Our calculations show that triplet O₂ abstracts a hydrogen radical from intermediate **13** via transition structure **TS_{13-14T}** with a barrier of 10.3 kcal/mol, leading to formation of the triplet complex **14T**. This species then undergoes intersystem crossing through a minimum energy crossing point (**MECP**) with a barrier of approximately 0.1 kcal/mol to afford the singlet complex **14**. Spin density analysis of **14T** indicates significant spin density on Pd (1.04) and on the HOO ligand (0.725), consistent with a formal Pd(I) oxidation state and radical character on the hydroperoxo ligand.

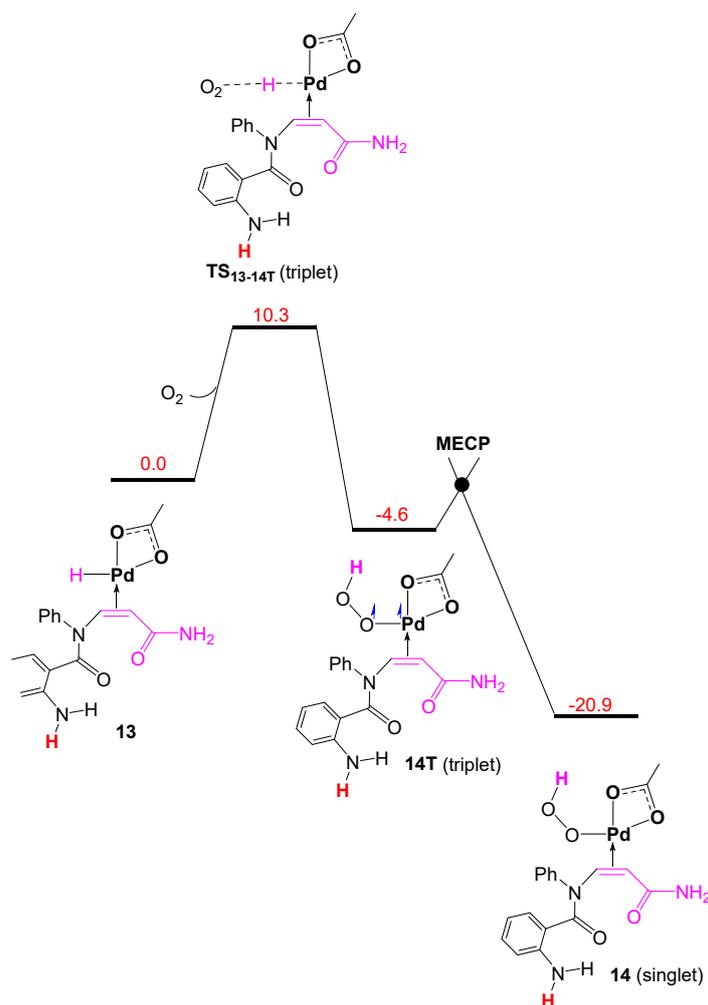


Figure S5. Computed free-energy profile for formation of the Pd–hydroperoxo species via reaction of triplet O₂ with the Pd(II)–H intermediate **13**. Relative free energies were calculated at the SMD/M06-L-D3/SDD,6-311+G(2d,p)//SMD/M06-L-D3/SDD,6-31G(d) level of theory in water and are reported in kcal/mol.

The minimum energy crossing point (MECPs), as reported in Fig. S5, was located using the code developed by Harvey and co-workers.⁷

7. Total energies for all of the calculated structures

Table S2. Total potential (E) and Gibbs free energies (G) of all structures optimized at the SMD/M06-L-D3/BS1 level of theory along with the total potential energies calculated by SMD/M06-L-D3/BS2 //SMD/M06-L-D3/BS1 in water solvent. BS1: SDD,6-31G(d) and BS2: SDD,6-311+G(2d,p).

Structure	E (SMD/M06-L-D3/BS1)	H (SMD/M06-L-D3/BS1)	G (SMD/M06-L-D3/BS1)	E ((SMD/M06-L-D3/BS2)// (SMD/M06-L-D3/BS1))
Pd ₃ OAc ₆	-1754.934508	-1754.586467	-1754.691269	-1755.331687
AcOH	-229.063181	-228.995997	-229.029175	-229.142043
CO ₂	-188.570787	-188.555488	-188.580433	-188.629726
O ₂	-150.304997	-150.297918	-150.321207	-150.354147
H ₂ O ₂	-151.527609	-151.497121	-151.523606	-151.590715
1a	-588.282935	-588.15213	-588.195643	-588.445679
2a	-287.565417	-287.441254	-287.476971	-287.64924
3a	-247.2713	-247.185674	-247.220789	-247.351833
4a	-933.394937	-933.087969	-933.153674	-933.65095
4'a	-934.589872	-934.259697	-934.329983	-934.854105
4''a	-933.362011	-933.057222	-933.125294	-933.623269
4'''a	-934.592479	-934.262669	-934.330385	-934.856858
5	-687.281276	-687.041484	-687.096333	-687.472015
6	-1272.251614	-1271.894061	-1271.979609	-1272.572789
TS ₆₋₈	-1272.232685	-1271.881263	-1271.966264	-1272.556284
TS ₆₋₇	-1272.241014	-1271.888839	-1271.973247	-1272.564256
7	-1272.241319	-1271.885844	-1271.971836	-1272.564756
8	-1272.233578	-1271.879231	-1271.962107	-1272.557138
9	-1290.451579	-1290.076024	-1290.160713	-1290.779266
TS ₉	-1290.417918	-1290.044849	-1290.129152	-1290.743915
TS ₉₋₁₀	-1290.424537	-1290.051011	-1290.135193	-1290.750816
10	-1290.458754	-1290.082046	-1290.165449	-1290.783304
11	-1290.457171	-1290.081929	-1290.164264	-1290.782548
12	-1290.441097	-1290.065612	-1290.152294	-1290.770212
TS ₁₂₋₁₃	-1290.424932	-1290.054075	-1290.139129	-1290.755896
13	-1290.440923	-1290.068663	-1290.154294	-1290.769778
14	-1440.805472	-1440.420799	-1440.511132	-1441.181157
15	-1669.894052	-1669.439754	-1669.542657	-1670.34425
TS ₁₅₋₁₆	-1669.888404	-1669.437724	-1669.53891	-1670.338801
16	-1669.888491	-1669.435422	-1669.539599	-1670.339287
17	-1518.329681	-1517.90921	-1518.003451	-1518.721576
TS ₁₇₋₁₈	-1518.310989	-1517.890161	-1517.98462	-1518.701008
18	-1518.352451	-1517.927622	-1518.017836	-1518.740944
TS ₁₈₋₁₉	-1518.345499	-1517.926145	-1518.01716	-1518.734784
19	-1518.351335	-1517.927913	-1518.01778	-1518.741186
20	-933.342663	-933.03628	-933.099413	-933.603364
TS ₂₁	-934.528877	-934.200384	-934.268161	-934.798267
21	-934.52893	-934.199538	-934.268824	-934.798779
TS ₂₂	-934.523509	-934.198707	-934.266228	-934.792641
22	-934.537616	-934.208157	-934.2774	-934.806332
TS _{22'}	-934.505467	-934.182121	-934.249519	-934.774769
22'	-934.548853	-934.219643	-934.286852	-934.817477
TS1a-5A	-875.825359	-875.56853	-875.626912	-876.071508

5A	-875.825429	-875.567553	-875.630511	-876.072338
(H2O)2	-152.832339	-152.779744	-152.811726	-152.913013
TSSB-5C	-1028.670948	-1028.362586	-1028.431249	-1028.991659
5B	-1028.679124	-1028.366512	-1028.438704	-1028.999733
5C	-1028.711192	-1028.399018	-1028.469388	-1029.03265
5D	-875.855532	-875.598364	-875.659588	-876.102982
5E	-875.859898	-875.60388	-875.667116	-876.107683
1a(tol)	-588.279712	-588.148834	-588.192486	-588.442613
2a(tol)	-287.566482	-287.442258	-287.478044	-287.650968
TS1a-5D(tol)	-875.811312	-875.554781	-875.613243	-876.058048
5D(tol)	-875.846673	-875.588517	-875.649506	-876.094501
1a(ACN)	-588.286224	-588.155489	-588.19908	-588.449611
2a(ACN)	-287.571116	-287.447008	-287.482726	-287.654928
TS1a-5D(ACN)	-875.824234	-875.56764	-875.626339	-876.072052
5D(ACN)	-875.85578	-875.598122	-875.659572	-876.103653
2 (X = NO2)	-492.073186	-491.944153	-491.986643	-492.216222
TS1a-5A (X = NO2)	-1080.314722	-1080.053335	-1080.118558	-1080.621597
2 (X = OMe)	-402.071674	-401.912163	-401.953928	-402.191021
TS1a-5A (X = OMe)	-990.335373	-990.04349	-990.108088	-990.617416
TSRE	-1290.370597	-1289.997102	-1290.081948	-1290.695206
TS13-14T	-1440.735711	-1440.359412	-1440.457089	-1441.112635
14T	-1440.769427	-1440.385868	-1440.481688	-1441.145606

8. Cartesian coordinates for all of the calculated structures

17

1a.out

```

C -2.77377100 -1.02742400 0.00258000
C -1.52428900 -1.62934200 0.00587500
C -0.38403200 -0.82382600 0.00110600
C -0.50578900 0.57378000 -0.00120600
C -1.77741200 1.16350800 -0.00523300
C -2.90870400 0.36734500 -0.00481900
H -3.66204800 -1.65517500 0.00509900
H -1.41934800 -2.71169800 0.01133900
H -1.84867000 2.24858200 -0.00971500
H -3.89674400 0.81947100 -0.00927300
C 0.68701100 1.39070300 0.00197400
O 0.75317800 2.60136300 0.00536200
O 1.90739300 0.70369200 0.00168800
N 0.88416600 -1.37864400 -0.00211500
C 2.04065400 -0.66788200 -0.00188600
O 3.15585100 -1.14793100 -0.00372800
H 0.98426900 -2.38883100 0.00043100

```

14

2a.out

```

C -1.16867400 -1.20107500 0.00310000
C 0.22204800 -1.20690000 -0.00276700

```

C	0.94055200	0.00013200	-0.00813400
C	0.22201700	1.20707400	-0.00276800
C	-1.16866000	1.20106000	0.00304800
C	-1.87874700	-0.00013000	0.00509300
H	-1.70305500	-2.15018100	0.01003000
H	0.76948600	-2.14929000	-0.00246100
H	0.76920400	2.14954700	-0.00241300
H	-1.70315300	2.15008000	0.01039100
H	-2.96656800	-0.00004500	0.01156900
N	2.32918400	-0.00011800	-0.08678400
H	2.75959100	0.83321100	0.29718300
H	2.75898600	-0.83346200	0.29775400

10

3a.out

C	-0.47810200	0.12078600	-0.00229000
C	0.78958700	-0.64596000	-0.00798100
O	-0.51739600	1.36123400	-0.00301000
C	1.97126900	-0.02868800	0.00652500
H	2.03024400	1.05891900	0.02229300
H	2.90801200	-0.58013800	0.00427200
H	0.72337500	-1.73408400	-0.02228000
N	-1.59490900	-0.63865600	-0.00575900
H	-2.50196600	-0.19349400	0.03794800
H	-1.55265900	-1.64730300	0.04464200

38

4''a.out

C	-2.71355800	-1.48362700	0.59829500
C	-3.02602900	-0.73697100	-0.67989000
O	-1.85273300	-2.37151000	0.66018800
C	-1.88612200	-0.74874600	-1.68128600
H	-3.89540800	-1.21804300	-1.14825900
N	-3.45038800	-1.11620000	1.66589900
H	-3.35898800	-1.62636700	2.53441600
H	-4.17836100	-0.41895900	1.59309900
C	4.15331600	0.52283800	0.44572100
C	3.64206200	-0.65911000	0.96332200
C	2.42474000	-1.18608300	0.50077500
C	1.71979700	-0.46897300	-0.49364400
C	2.24987900	0.72182300	-1.00010500
C	3.46452200	1.22255200	-0.54728600
H	5.10417600	0.89928600	0.81923500
H	4.18274100	-1.19984900	1.73913700
H	1.69592500	1.25436300	-1.77239200
H	3.86735600	2.14413200	-0.96035700
C	0.46019900	-1.04051700	-1.04168600
O	0.43229300	-2.21675400	-1.44288200
N	1.88483600	-2.31963400	1.08709800
N	-0.63392900	-0.22016700	-1.12397100
H	2.56942700	-2.90757200	1.54768100
H	1.28079300	-2.85663900	0.47467900
H	-1.66841000	-1.76447400	-2.01476500
H	-2.16779100	-0.15740700	-2.56080700
C	-0.72872400	1.01900300	-0.41726200

C	-1.12992200	2.17183800	-1.09381500
C	-0.49595800	1.06040300	0.96016700
C	-1.27128400	3.36858500	-0.39601200
H	-1.32273200	2.12800500	-2.16446300
C	-0.62584600	2.26280300	1.64816600
H	-0.21545600	0.14597700	1.48243100
C	-1.01319300	3.41959200	0.97294700
H	-1.57879700	4.26654600	-0.92805400
H	-0.43650700	2.29099000	2.71931700
H	-1.12095000	4.35723900	1.51411100
H	-3.34041100	0.28843200	-0.44707000

38

4'a.out

C	-4.51717400	-1.06532800	0.17203200
C	-4.10260900	-0.08099900	1.24141100
O	-3.88050000	-1.21643700	-0.88200700
C	-3.14057600	0.98481800	0.75967400
H	-4.99402700	0.39500000	1.66640200
N	-5.62583400	-1.77835300	0.44854600
H	-5.91830800	-2.51295800	-0.18202400
H	-6.12025300	-1.67084400	1.32339300
C	0.18229300	3.40521200	-0.34322300
C	-0.86831600	2.61041700	0.09445400
C	-0.83939200	1.21166300	-0.06769300
C	0.30905100	0.63675900	-0.67985900
C	1.34930600	1.46410300	-1.11865500
C	1.29895800	2.84278600	-0.96299700
H	0.11920000	4.48387200	-0.20844300
H	-1.73196000	3.07809300	0.55952600
H	2.20747800	1.00733300	-1.60935900
H	2.11224700	3.46815900	-1.32253500
C	0.36846100	-0.81778100	-0.94585000
O	-0.62247000	-1.45491100	-1.34530800
N	-1.85234500	0.40759500	0.41292500
N	1.56839300	-1.46735800	-0.82279700
H	-1.95252100	-0.45196700	-0.11935700
H	1.56216400	-2.39950200	-1.22649400
H	-3.57936900	1.53628300	-0.09006200
H	-3.00141600	1.71242400	1.56729300
C	2.73036000	-1.12009400	-0.09920700
C	3.96310700	-1.58933100	-0.56333400
C	2.67336500	-0.38150800	1.08826000
C	5.12853700	-1.30544600	0.14213000
H	3.99895100	-2.17543400	-1.48014500
C	3.84623000	-0.08814200	1.77563100
H	1.71277600	-0.04792800	1.47378400
C	5.07839600	-0.54519000	1.30884600
H	6.08144200	-1.67686500	-0.22966000
H	3.79098600	0.48914800	2.69650900
H	5.99063500	-0.31798000	1.85616100
H	-3.64573600	-0.65089300	2.06308000

36

4a.out

C	0.41753300	3.04475600	0.45417400
C	0.05358800	1.60026700	0.70352300
O	0.85105300	3.43888100	-0.63997300
C	-0.02638700	0.79617000	-0.59336000
N	0.23803400	3.87187800	1.49891800
H	0.49902900	4.84578900	1.41816600
H	-0.11018200	3.53688900	2.38668400
H	-0.70533900	1.30371000	-1.28537700
N	-0.58700900	-0.53875000	-0.33450300
C	0.21391500	-1.54452800	0.16311000
C	-2.00967000	-0.61037500	-0.22378400
O	-0.25526400	-2.61143500	0.58461300
C	1.66231800	-1.29601000	0.08123400
C	-2.62331900	-0.94355300	0.98643300
C	-2.78968600	-0.29278400	-1.33758300
C	2.15492800	-0.19541200	-0.65041200
C	2.55765100	-2.20099100	0.66172400
C	-4.01233300	-0.97648900	1.06930300
H	-2.01153300	-1.17033700	1.85568600
C	-4.17818800	-0.31759700	-1.24369000
H	-2.30343300	-0.03210000	-2.27630000
N	1.24844500	0.64710100	-1.27128100
C	3.54013300	-0.02668700	-0.78669300
C	3.92711000	-2.02317600	0.53703400
H	2.15050000	-3.04628500	1.21298400
C	-4.79359100	-0.66455400	-0.04239400
H	-4.48540200	-1.23689900	2.01406700
H	-4.77923800	-0.07112900	-2.11651300
C	4.40957500	-0.93201700	-0.19546300
H	3.91869100	0.82193900	-1.35389700
H	4.61814500	-2.72448800	0.99808600
H	-5.87900200	-0.68773800	0.02890700
H	5.48268400	-0.78265000	-0.30140200
H	-0.90599300	1.54495400	1.23474800
H	1.62649700	1.56373700	-1.49817800
H	0.80049400	1.15132800	1.37435300

36

4"a.out

C	-3.38152400	-0.40265100	0.50351900
C	-2.86838400	-1.57002700	-0.21901600
O	-2.65946800	0.44201800	1.06395000
C	-1.58261300	-1.81565600	-0.54210600
H	-3.57983000	-2.35637500	-0.46079000
N	-4.73454900	-0.31725700	0.54788500
H	-5.15991000	0.38358400	1.13976700
H	-5.32257900	-1.06021100	0.19601500
H	-1.32110300	-2.79384900	-0.94463100
N	-0.49100500	-0.95791500	-0.42466300
C	-0.60742600	0.42654900	-0.72731100
C	0.78930100	-1.56480500	-0.27081900
O	-1.43423000	0.80548700	-1.55754700
C	0.30013800	1.33249700	-0.01337300
C	1.89038000	-1.11363600	-1.00665400
C	0.92680400	-2.65093000	0.59701100

C	0.71666700	2.55314800	-0.60995700
C	0.71042500	1.03026900	1.29721300
C	3.12392500	-1.73493900	-0.84947700
H	1.77539100	-0.28762400	-1.70674100
C	2.16205300	-3.27881100	0.73139100
H	0.06694200	-2.98830500	1.17352600
N	0.39465700	2.88124800	-1.90428500
C	1.56335300	3.40001700	0.13211200
C	1.52218100	1.88570200	2.02011200
H	0.35042400	0.10973500	1.75336600
C	3.26593100	-2.81946000	0.01665500
H	3.97654900	-1.37809600	-1.42345900
H	2.26099400	-4.12346200	1.41008300
H	-0.47323700	2.48905900	-2.24712600
H	0.52534100	3.85644200	-2.14203900
C	1.95591900	3.07356700	1.41780700
H	1.89727900	4.32897900	-0.32795800
H	1.81366200	1.64016000	3.03805200
H	4.23234800	-3.30585400	0.12941500
H	2.60081000	3.75822800	1.96609300

28

5.out

C	-3.08605000	-1.75631000	-0.01016700
C	-2.09409600	-1.61809600	0.94718900
C	-1.25171600	-0.49070900	0.97398500
C	-1.44358900	0.50560700	-0.01449400
C	-2.48173200	0.36338200	-0.94561900
C	-3.29306200	-0.76071800	-0.96922500
H	-3.71397200	-2.64561800	-0.00037100
H	-1.95276400	-2.38575200	1.70719800
H	-2.62426300	1.16024500	-1.67407800
H	-4.07703900	-0.86051800	-1.71581800
C	-0.66875000	1.76995200	-0.07587600
O	-1.23927200	2.86437400	-0.19695400
N	-0.26155900	-0.41796300	1.93592200
N	0.69717900	1.72816100	0.02810900
H	-0.46244600	-0.95129400	2.77340600
H	0.07896000	0.50968200	2.15711900
C	1.58584200	0.64951100	-0.17413400
C	1.30940300	-0.38108800	-1.07829300
C	2.79559000	0.65066800	0.52754800
C	2.22003800	-1.42133500	-1.23635300
H	0.39173500	-0.36377000	-1.66102300
C	3.70826200	-0.38269500	0.34544500
H	3.00855900	1.46343400	1.22019700
C	3.42004200	-1.43107900	-0.52715700
H	1.99380600	-2.22188100	-1.93803900
H	4.64564300	-0.37156900	0.89815700
H	4.13040300	-2.24376300	-0.66247300
H	1.12511900	2.64188500	0.14604600

43

6.out

Pd	-0.89125000	-0.36863000	0.30769500
----	-------------	-------------	------------

O	-2.26278500	-1.74877100	-0.35845100
C	-2.57430700	-1.60081400	-1.61736500
O	-2.08284100	-0.74391800	-2.36746600
O	-3.20173400	1.44726800	0.01508000
C	-3.15778500	1.09011200	1.20332400
O	-2.24789300	0.30107400	1.70138100
C	-3.62909700	-2.56367400	-2.09244800
H	-4.60840400	-2.22951100	-1.73009300
H	-3.65768400	-2.59766900	-3.18406100
H	-3.46155200	-3.56838200	-1.69369000
C	-4.20362700	1.52149600	2.19536600
H	-3.78799100	1.63618300	3.20018300
H	-4.67346100	2.45578500	1.87786600
H	-4.98200300	0.75082100	2.24736600
C	1.36707000	0.08302600	1.69695700
N	0.57576600	1.04353400	0.98097600
O	1.31696200	0.05756500	2.91778000
N	0.61558600	-1.04281400	-0.99031500
H	0.28434400	-1.84751000	-1.52714800
H	0.75136900	-0.29635700	-1.68072300
C	1.87544500	-1.37483400	-0.35121200
C	2.72742000	-2.27803500	-0.97753400
C	2.21500600	-0.84260600	0.90428900
C	3.92727000	-2.64758700	-0.37592200
H	2.43721200	-2.69973500	-1.93787300
C	3.41728600	-1.23967200	1.50389200
C	4.27541500	-2.12529300	0.86719800
H	4.58331400	-3.35370900	-0.87934900
H	3.66836800	-0.82913500	2.47913300
H	5.20826900	-2.41436400	1.34433900
C	1.17163700	1.82725500	-0.09158400
C	2.52792300	2.14613300	-0.06120800
C	0.35111900	2.27377900	-1.12704600
C	3.06802700	2.90890500	-1.09360900
H	3.15488600	1.81368200	0.76416700
C	0.90046500	3.04478800	-2.14713800
H	-0.70674500	2.00738300	-1.12621600
C	2.25906100	3.35669200	-2.13565500
H	4.12649400	3.15776400	-1.07494200
H	0.26315000	3.39437800	-2.95602900
H	2.68727800	3.95202300	-2.93891700
H	0.08756200	1.63652200	1.65893500

43

7.out

Pd	1.03517000	-0.03055500	-0.31155600
O	2.49671100	1.09383400	-1.26262000
C	2.50202700	2.36072100	-0.95957700
O	1.71254500	2.90164000	-0.16821200
O	1.41668400	-2.81569400	1.39814400
C	2.54722500	-2.24105400	1.09480800
O	2.64113000	-1.16895900	0.45320600
C	3.59187700	3.14198300	-1.64584200
H	3.67558800	2.86389200	-2.70071000
H	3.41278100	4.21638600	-1.55999500

H	4.55405300	2.91119300	-1.17391500
C	3.76494300	-2.93538100	1.58347800
H	4.66333200	-2.51684300	1.12871800
H	3.82581600	-2.81771100	2.67147800
H	3.69682300	-4.00706000	1.37653100
C	-0.78620600	-0.22517300	1.54730500
N	-0.49285200	-1.19024800	0.57076800
O	-0.35463900	-0.34380100	2.69775900
N	-0.53391500	1.10424100	-1.07423100
H	-0.16457600	1.87355700	-1.63686700
H	-1.04868500	0.49431500	-1.71973300
C	-1.43457700	1.63661600	-0.06484100
C	-2.12041800	2.81711400	-0.32814700
C	-1.57434500	0.99130100	1.17196900
C	-2.97347300	3.35558200	0.63211200
H	-1.97428100	3.31775200	-1.28379800
C	-2.42038800	1.55635500	2.13129700
C	-3.12887300	2.72134700	1.86243700
H	-3.50631100	4.27910000	0.41786900
H	-2.51502700	1.05972100	3.09479000
H	-3.78968600	3.14176400	2.61662900
C	-1.49821400	-1.60295400	-0.32939100
C	-2.85578000	-1.61083100	0.02963800
C	-1.12709000	-2.10564700	-1.58769100
C	-3.81094400	-2.09926500	-0.85706300
H	-3.15918700	-1.25588500	1.01360900
C	-2.08959600	-2.59175800	-2.46506800
H	-0.07117200	-2.09780700	-1.86258400
C	-3.43820900	-2.58798200	-2.10788400
H	-4.85815400	-2.09997500	-0.56017600
H	-1.78173100	-2.97379400	-3.43661500
H	-4.19040700	-2.96671000	-2.79624200
H	0.61319800	-2.23629900	1.07536400

43

8.out

Pd	-1.02385000	-0.04717400	0.11147100
O	-1.67987200	-3.12886700	-0.64696400
C	-2.74580900	-2.37049700	-0.73463100
O	-2.71970500	-1.12754600	-0.61176200
O	-2.84040300	2.06501100	-0.80575400
C	-2.99049600	1.98843600	0.42775600
O	-2.33459900	1.16908500	1.19341900
C	-4.01289600	-3.09383300	-0.99894400
H	-4.15542800	-3.87227400	-0.24258900
H	-4.86097600	-2.40885700	-0.99279200
H	-3.94993000	-3.59613300	-1.97002600
C	-4.00185500	2.84357000	1.14309100
H	-3.67267100	3.10135800	2.15365300
H	-4.20878800	3.75508200	0.57629200
H	-4.94024000	2.28358700	1.23609400
C	1.23205300	-0.14659900	1.73072300
N	0.60867400	0.93570800	0.96672900
O	1.17165000	-0.09994200	2.95293900
N	0.29004000	-1.29006000	-0.83195500

H	-0.85037600	-2.53402400	-0.58294700
H	0.25615300	-1.24133200	-1.85162200
C	1.57431300	-1.48338600	-0.38268300
C	2.52045800	-2.16264900	-1.18116000
C	1.95789600	-1.13536700	0.94146400
C	3.71904500	-2.59628400	-0.64350900
H	2.26168500	-2.39289400	-2.21361000
C	3.16115000	-1.62504100	1.47915000
C	4.03937000	-2.35754800	0.70163000
H	4.41655200	-3.14178400	-1.27693800
H	3.41476600	-1.35498600	2.50294900
H	4.98045000	-2.70986600	1.11586000
C	1.44457700	1.66266900	0.01214700
C	2.81163400	1.80337300	0.24591900
C	0.84728200	2.24748600	-1.10213400
C	3.58796100	2.51810400	-0.66273900
H	3.26831800	1.36574600	1.13154600
C	1.63079400	2.96916600	-1.99840400
H	-0.22599500	2.13318700	-1.25831700
C	3.00214900	3.09790400	-1.78583200
H	4.65583700	2.62236300	-0.48465200
H	1.16511800	3.42414900	-2.86968800
H	3.61374000	3.65260500	-2.49395500
H	0.19554500	1.58558200	1.64356300

45

9.out

Pd	-0.98902400	-0.29804200	0.18638300
O	-2.47072100	-1.66207200	-0.40956400
C	-2.25055100	-2.76555400	-1.05749600
O	-1.14218400	-3.18904800	-1.43185700
C	-3.50988900	-3.54160500	-1.34861400
H	-4.16072900	-2.95809400	-2.00922400
H	-3.27826100	-4.49547200	-1.82811800
H	-4.07074800	-3.72301000	-0.42605400
C	1.26076000	0.23700200	1.57448300
N	0.46695000	1.08460300	0.78249500
O	1.18544100	0.27603300	2.80486700
N	0.61130900	-1.07726800	-0.98699200
H	0.20162100	-1.92582900	-1.40810400
H	0.78287900	-0.39408300	-1.73118900
C	1.83846000	-1.39500800	-0.28898800
C	2.67424000	-2.37705200	-0.81313000
C	2.15814100	-0.76828100	0.92447200
C	3.84700700	-2.72567800	-0.14777500
H	2.39517000	-2.87247800	-1.74138300
C	3.32984000	-1.14489800	1.58998200
C	4.17947000	-2.10463100	1.05448300
H	4.49378200	-3.49285700	-0.56746700
H	3.56544700	-0.66155900	2.53596300
H	5.09261300	-2.37684700	1.57845100
C	1.08574100	1.74833100	-0.28327900
C	2.44679200	2.11121400	-0.23878300
C	0.32073100	2.17505800	-1.38642600
C	3.00970700	2.86778500	-1.26126100

H	3.05487500	1.82448800	0.61862200
C	0.89667300	2.92384700	-2.40544300
H	-0.73440500	1.89979700	-1.42956400
C	2.24575400	3.27660700	-2.35358400
H	4.06186100	3.14080700	-1.19805900
H	0.28208900	3.23551800	-3.24840300
H	2.69372800	3.86555200	-3.15070400
O	-1.97900300	2.96745100	1.62333300
C	-2.60392300	2.27112200	0.81446800
C	-2.76300800	0.79365600	0.96866000
N	-3.24527200	2.77961700	-0.25737600
C	-2.16823800	0.08999900	1.99487700
H	-3.55220200	0.32245700	0.38299900
H	-3.16902200	3.76767200	-0.46197100
H	-3.70884400	2.18421800	-0.93056400
H	-1.50866000	0.59764200	2.69813200
H	-2.51151600	-0.90703100	2.26203300

45

10.out

Pd	0.92937200	-0.02275800	-0.46594500
O	2.68391000	0.56844100	-1.43821000
C	3.45686300	1.29746300	-0.69218900
O	3.16951700	1.68796700	0.45456500
C	4.79518000	1.62267900	-1.30264800
H	4.75668000	1.64485100	-2.39510200
H	5.17314600	2.57650300	-0.92462400
H	5.51012000	0.84252200	-1.01134800
C	-0.79815600	0.13539000	1.47564700
N	-0.64308200	-0.97519800	0.57152400
O	-0.29763100	0.13379400	2.59143600
N	-0.14348300	1.87683700	-0.84045700
H	0.50639700	2.54786800	-0.42443600
H	-0.23681700	2.15356500	-1.81806800
C	-1.42118900	1.98409300	-0.17887700
C	-2.37757000	2.88530400	-0.64473500
C	-1.68922500	1.22183300	0.97012500
C	-3.57615900	3.05907400	0.03909600
H	-2.16060400	3.46877100	-1.53799700
C	-2.87590400	1.44427600	1.67922400
C	-3.81897100	2.35221900	1.21554100
H	-4.31157200	3.76635900	-0.33759600
H	-3.06523800	0.86243800	2.57954100
H	-4.74569400	2.49903000	1.76489300
C	-1.80326100	-1.38197400	-0.20336100
C	-2.96302200	-1.74213700	0.48302500
C	-1.74102800	-1.45995200	-1.59203500
C	-4.07615400	-2.16758700	-0.23532100
H	-2.98812400	-1.68503500	1.57042800
C	-2.85843800	-1.89433300	-2.30202000
H	-0.82046700	-1.17405700	-2.10281000
C	-4.02586400	-2.24371700	-1.62671300
H	-4.98459000	-2.44158600	0.29651500
H	-2.81403100	-1.95395500	-3.38717300
H	-4.89818700	-2.57670900	-2.18474600

O	2.71511900	-1.21135700	2.26799500
C	2.77223000	-1.56753700	1.07650400
C	1.57420800	-1.84573200	0.25732400
N	3.97028200	-1.74473500	0.44728400
C	0.28785200	-2.09643300	1.00530500
H	1.75039400	-2.49924600	-0.60255800
H	4.77260300	-1.29614600	0.87335600
H	3.97971600	-1.77225100	-0.56518400
H	-0.20346200	-3.03925900	0.75254900
H	0.40693100	-2.02344400	2.08972100

45

11.out

Pd	-1.34733500	0.02818000	-0.33259000
O	-3.11341000	-0.86458100	-1.08392500
C	-2.48731000	-1.75205400	-1.77708200
O	-1.22117800	-1.76688000	-1.77388400
C	-3.27667300	-2.76265300	-2.53706500
H	-4.25105700	-2.36535000	-2.83293900
H	-2.72653800	-3.10308600	-3.41807500
H	-3.45122800	-3.63392800	-1.89423600
C	0.95058000	-0.07110400	1.35102300
N	0.37674100	1.00344900	0.53955600
O	0.68195600	-0.10631000	2.55112900
N	2.61239300	-1.95394600	2.81924600
H	2.13853200	-1.21339200	3.31723600
H	3.40586800	-2.38340800	3.27599300
C	2.62935000	-1.91706500	1.45936800
C	3.48883800	-2.81104100	0.77948000
C	1.80414800	-1.04814700	0.67869700
C	3.50466200	-2.89060900	-0.59594700
H	4.13242900	-3.45412000	1.37770800
C	1.84201400	-1.17061500	-0.72918200
C	2.66218300	-2.07588800	-1.36830800
H	4.17337000	-3.59921700	-1.08133900
H	1.18611300	-0.54648800	-1.33097800
H	2.65414800	-2.15254600	-2.45240800
C	1.28215800	1.71760000	-0.34717200
C	2.55970700	2.04762700	0.10313800
C	0.84350700	2.12725900	-1.60417800
C	3.41070300	2.77214400	-0.72734400
H	2.88544200	1.73925000	1.09565800
C	1.69716100	2.86146700	-2.42288900
H	-0.15977200	1.85252800	-1.93422500
C	2.98351400	3.17917300	-1.98979200
H	4.41065200	3.02251800	-0.37971800
H	1.35614800	3.17720600	-3.40645100
H	3.65201000	3.74450400	-2.63532900
O	-2.42178100	0.51416800	2.94824800
C	-2.83016100	0.98389000	1.87141800
C	-1.92739400	1.57291000	0.85261300
N	-4.15158900	1.01029500	1.55648000
C	-0.54133100	1.94832300	1.29821600
H	-2.41127600	2.28909700	0.17989300
H	-4.78313600	0.44617700	2.11083700

H	-4.43738500	1.21760100	0.60810400
H	-0.26170900	2.96746700	1.02216400
H	-0.37666200	1.80183800	2.36776500

45

12.out

Pd	2.48115900	-0.12207600	-0.48495200
O	4.18920800	-0.84488400	0.56224200
C	4.76471200	0.30650000	0.55519300
O	4.19235300	1.28503900	-0.01414200
C	6.07540900	0.46482300	1.24570000
H	6.67387900	-0.44679500	1.16770500
H	6.63035600	1.31433100	0.84029300
H	5.89612500	0.65296800	2.31107300
C	-1.86892800	-0.94387900	-0.64267300
N	-0.88486700	0.00936300	-0.78498000
O	-1.71338500	-2.06557000	-1.15452500
N	-4.54081200	-1.82924100	-1.37399900
H	-3.79190700	-1.83564100	-2.05366800
H	-5.45971900	-1.74281600	-1.78965300
C	-4.34306800	-1.06756600	-0.24336600
C	-5.44982600	-0.74581000	0.56617500
C	-3.06359300	-0.61409300	0.16566100
C	-5.29480100	-0.05186900	1.75392700
H	-6.43827100	-1.06831900	0.24140300
C	-2.93160300	0.07855800	1.37935100
C	-4.02681300	0.35484300	2.18201700
H	-6.17283400	0.17163100	2.35759800
H	-1.93842400	0.39401400	1.69363800
H	-3.89915100	0.88200300	3.12411700
C	-1.06233700	1.40399600	-0.53850200
C	-2.13620700	2.08493100	-1.11617900
C	-0.15339300	2.08748800	0.27313600
C	-2.30824600	3.44245200	-0.86397300
H	-2.83296100	1.54388800	-1.75422200
C	-0.32222700	3.44958700	0.50466000
H	0.67405400	1.54289000	0.73297600
C	-1.40183100	4.12929900	-0.05735700
H	-3.14919100	3.96738500	-1.31232200
H	0.38677100	3.97690200	1.13964500
H	-1.53526300	5.19235000	0.13101600
O	0.24268400	-1.36213000	1.49515400
C	0.71262000	-2.07913500	0.59480900
C	1.09056800	-1.56391900	-0.74775500
N	0.98808900	-3.38632600	0.78493900
C	0.35220200	-0.45400500	-1.40278400
H	1.46738600	-2.32163300	-1.43980800
H	0.78781500	-3.81209800	1.68059600
H	1.32692700	-3.97519900	0.03657400
H	1.01555900	0.49340000	-1.46858200
H	0.20595500	-0.66318100	-2.47040200

45

13.out

Pd	2.43284600	-0.39777600	-0.29315700
O	1.59030300	0.33656200	1.73942700

C	2.69617200	0.92767900	1.90897300
O	3.62909500	0.81935700	1.02632500
C	2.93595800	1.79056600	3.10279800
H	2.27537200	1.51285100	3.92784700
H	3.97998600	1.73981800	3.42382100
H	2.72389000	2.83272400	2.83418800
C	0.75361800	-2.74888500	-0.32825400
C	1.26043600	-1.80067900	-1.35667100
O	0.27510100	-2.36991800	0.75382200
C	0.70674800	-0.52783700	-1.62414300
H	1.84355900	-2.23217400	-2.16828100
N	0.89941700	-4.04839600	-0.64465400
H	0.60461900	-4.75834000	0.01340600
H	1.28204800	-4.34197500	-1.53326200
H	3.38038800	-0.60326200	-1.49490500
H	1.06826000	0.00770400	-2.50143000
N	-0.45284100	-0.00281000	-1.07494500
C	-1.54153600	-0.87799000	-0.72094000
C	-0.68282500	1.39700100	-1.24876900
O	-1.71101800	-1.89834600	-1.39176200
C	-2.37942700	-0.47338300	0.39564300
C	-1.93208700	1.85587000	-1.67834700
C	0.35410700	2.30550300	-1.01955900
C	-3.67965700	-1.04024300	0.56017400
C	-1.91612300	0.46290200	1.34559000
C	-2.14121400	3.21846300	-1.85812700
H	-2.73230800	1.14712200	-1.88333700
C	0.13813000	3.66601800	-1.22109300
H	1.32357700	1.94540900	-0.67210100
N	-4.17300100	-2.01679000	-0.24723800
C	-4.47511200	-0.57815700	1.63315200
C	-2.69620700	0.87016300	2.40700500
H	-0.90818900	0.85634000	1.23812300
C	-1.10937100	4.12900700	-1.63252700
H	-3.11568200	3.56690500	-2.19367000
H	0.95090200	4.36630400	-1.03994100
H	-3.67345200	-2.23727700	-1.09802600
H	-5.17453700	-2.15551600	-0.24965600
C	-3.99526800	0.35110100	2.53190500
H	-5.47756400	-0.98858500	1.74315900
H	-2.31155300	1.58237900	3.13218300
H	-1.27723300	5.19353600	-1.77989300
H	-4.63393500	0.67587600	3.35151300

47

14.out

Pd	2.26299900	-0.31427100	0.17410900
O	0.90787100	0.13893200	1.77881900
C	1.60325600	1.13761700	2.17933500
O	2.73835900	1.35246300	1.64593400
C	1.03764300	2.05369700	3.20709400
H	0.34984100	1.52385300	3.87198400
H	1.82708100	2.53882900	3.78680000
H	0.46594600	2.83744500	2.69226600
C	0.64041200	-2.78264900	-0.16466600

C	1.27291300	-1.75639100	-1.03562100
O	-0.10696900	-2.50356400	0.78527100
C	0.70517000	-0.51311900	-1.41114100
H	2.03847500	-2.12108100	-1.72044400
N	0.98337700	-4.04924100	-0.46963700
H	0.62560800	-4.80990600	0.09361500
H	1.59122800	-4.26857800	-1.24706100
H	1.22299900	0.05565200	-2.18398500
N	-0.54322400	-0.02862200	-1.10237800
C	-1.64943900	-0.93424900	-0.86722300
C	-0.79396700	1.36012600	-1.32317900
O	-1.71042700	-1.94895300	-1.56256500
C	-2.61776700	-0.55251700	0.14404500
C	-1.99567700	1.76831300	-1.91026700
C	0.16804800	2.30772300	-0.96335700
C	-3.88845800	-1.20524200	0.19911700
C	-2.32049700	0.44150400	1.10453300
C	-2.23420800	3.12175200	-2.11844100
H	-2.73398400	1.02811600	-2.21310500
C	-0.07725800	3.65930100	-1.18987500
H	1.09893000	1.98868900	-0.49509600
N	-4.23336800	-2.22959800	-0.62178000
C	-4.81601000	-0.77697300	1.17698800
C	-3.22849400	0.81648200	2.07068200
H	-1.33849500	0.90665400	1.08944100
C	-1.27883800	4.07256300	-1.76008000
H	-3.17056500	3.43203900	-2.57705300
H	0.67525500	4.39146200	-0.90436200
H	-3.63811200	-2.44625800	-1.40957100
H	-5.21395100	-2.46479000	-0.69290500
C	-4.49374100	0.20547700	2.08805900
H	-5.79266000	-1.25729700	1.20258500
H	-2.96808700	1.57491800	2.80479000
H	-1.47030100	5.13005700	-1.92760400
H	-5.23054300	0.50203100	2.83251600
O	3.74752100	-0.42805400	-1.14649600
O	4.82566800	0.18810800	-0.44567600
H	4.70118100	1.13489800	-0.65359100

55

15.out

O	3.28735900	0.52937600	1.21898700
C	4.29512700	1.19439700	0.90985100
O	4.68619800	1.38126900	-0.32944400
C	5.14793700	1.84690900	1.93459500
H	4.76345100	1.66151300	2.93778700
H	6.17329000	1.47157300	1.85408500
H	5.18524900	2.92483200	1.74545000
C	-0.03539000	-2.49732900	-0.93772100
C	0.55628700	-1.30293800	-1.59782300
O	-0.91968700	-2.45396800	-0.07209200
C	0.06241100	0.01768900	-1.59634300
H	1.25614700	-1.51267200	-2.40623700
N	0.51369200	-3.66025500	-1.35439500
H	0.26314000	-4.51716100	-0.87810400

H	1.30313500	-3.68002500	-1.98645500
H	0.57392700	0.74530400	-2.22839800
N	-1.11675400	0.45962800	-1.04993200
C	-2.29377400	-0.38466800	-1.08818100
C	-1.26263200	1.86113900	-0.82161600
O	-2.45432100	-1.10002000	-2.07486300
C	-3.21867800	-0.27384300	0.02886500
C	-2.44670300	2.51411200	-1.18005500
C	-0.20309700	2.58482600	-0.26779900
C	-4.56819100	-0.71330700	-0.11052900
C	-2.77979000	0.21425600	1.27700400
C	-2.56958900	3.88178900	-0.96494500
H	-3.26096400	1.95782600	-1.64105900
C	-0.33285700	3.95709200	-0.07288700
H	0.71453500	2.07071900	0.01992700
N	-5.07600200	-1.16281600	-1.29519400
C	-5.42059900	-0.60541900	1.00914300
C	-3.62531600	0.28865300	2.36538100
H	-1.73592100	0.50147800	1.38400800
C	-1.51579000	4.60920800	-0.41232000
H	-3.49246100	4.38347800	-1.24779700
H	0.49583500	4.51381000	0.35953400
H	-4.41296100	-1.53719000	-1.96128000
H	-5.96375300	-1.64533200	-1.24343000
C	-4.96006700	-0.11767600	2.21584100
H	-6.45459600	-0.92961500	0.90217100
H	-3.25907000	0.65058500	3.32286300
H	-1.61646900	5.68010600	-0.25090700
H	-5.64340400	-0.06160600	3.06147100
O	3.14703700	-0.18061700	-1.77259700
O	4.01743200	-1.32727900	-1.61274500
H	3.51291700	-2.02091900	-2.07999800
Pd	1.84795700	-0.31870400	-0.21609500
O	0.56239900	-0.35899600	1.41376300
C	0.74587800	-1.41184900	2.14995100
O	1.61709000	-2.27265900	1.92648500
C	-0.21725700	-1.54320200	3.29784400
H	-1.12546900	-2.04184200	2.93512900
H	0.21021500	-2.15492200	4.09663800
H	-0.51522700	-0.56778300	3.69387400
H	4.08036400	0.85643800	-0.96175700

55

16.out

O	3.25202600	0.49517400	1.23995800
C	4.27776600	1.18053100	0.88656800
O	4.63362700	1.39026000	-0.30601800
C	5.06928200	1.78946300	2.00517400
H	5.15624600	1.09497200	2.84527000
H	6.06201900	2.09308000	1.66543000
H	4.54077300	2.67766000	2.37102000
C	-0.01391300	-2.48687300	-0.94462200
C	0.58600200	-1.28306300	-1.57810600
O	-0.90991200	-2.45309400	-0.09065300
C	0.07322800	0.02952200	-1.58124800

H	1.29427900	-1.48347900	-2.38180700
N	0.53902300	-3.64416400	-1.36975600
H	0.27660800	-4.50835500	-0.91342500
H	1.33284100	-3.65764600	-1.99650100
H	0.60656400	0.77363400	-2.17490700
N	-1.11025100	0.46272200	-1.05364700
C	-2.28645600	-0.39183800	-1.09911600
C	-1.26909900	1.86327300	-0.82271100
O	-2.43785300	-1.09428600	-2.09528400
C	-3.21425900	-0.29028000	0.01343400
C	-2.45063700	2.50922500	-1.20011800
C	-0.22510900	2.58822000	-0.24216400
C	-4.55899600	-0.74409100	-0.13238100
C	-2.78750000	0.20719100	1.26268300
C	-2.58562900	3.87492200	-0.97955800
H	-3.25208800	1.95001800	-1.67970200
C	-0.36708600	3.95834200	-0.04172900
H	0.68786700	2.07640100	0.06387100
N	-5.05492800	-1.20380700	-1.31646100
C	-5.41907500	-0.64049700	0.98226200
C	-3.64015000	0.27704300	2.34512800
H	-1.74770000	0.50692800	1.37488900
C	-1.54717500	4.60475700	-0.40152500
H	-3.50576800	4.37311000	-1.27685300
H	0.44853600	4.51729100	0.41197200
H	-4.38720100	-1.56529000	-1.98480100
H	-5.94178000	-1.68849200	-1.27224400
C	-4.97019700	-0.14363300	2.18911800
H	-6.44907200	-0.97539600	0.87048900
H	-3.28367400	0.64629100	3.30343400
H	-1.65812100	5.67378000	-0.23459400
H	-5.65887400	-0.09083500	3.03057300
O	3.22840600	-0.09487100	-1.76115400
O	4.09829300	-1.26659700	-1.74725600
H	3.60565400	-1.84743200	-2.35894700
Pd	1.87341500	-0.29702600	-0.16832600
O	0.56391600	-0.36980300	1.40235700
C	0.72184500	-1.43422800	2.13690400
O	1.58589600	-2.30083600	1.93048700
C	-0.27288800	-1.54785800	3.25868200
H	-1.18425000	-2.02011700	2.87024900
H	0.12294300	-2.17621100	4.06060000
H	-0.55409900	-0.56826300	3.65597800
H	3.85940500	0.58991800	-1.24750500

51

17.out

Pd	1.27440200	-0.91873600	0.05627800
O	3.00703900	-2.70385100	-1.43045100
C	3.23386300	-1.56043000	-1.85325000
O	2.60984600	-0.48903600	-1.44658000
C	4.30303900	-1.29194200	-2.87604600
H	4.10837800	-0.38209200	-3.44908800
H	5.26004800	-1.16406000	-2.35639100
H	4.40166100	-2.14545700	-3.55207200

C	-0.97920800	-1.95753300	0.23717600
C	-0.52601900	-1.28581400	-0.99368100
O	-0.40519300	-1.54214700	1.30198100
C	-0.36104500	0.11561300	-1.09397400
H	-0.42814500	-1.86573200	-1.90940400
N	-1.78221400	-3.00529100	0.20554700
H	-2.05069100	-3.45909100	1.07191600
H	-2.30998800	-3.21758500	-0.63337200
H	0.11081500	0.48115900	-2.00613500
N	-0.89190500	1.11081400	-0.31459400
C	-1.90368000	0.89482300	0.69082100
C	-0.29606000	2.41283300	-0.37465100
O	-1.75887500	1.43529600	1.77993400
C	-3.05703900	0.06745200	0.33869000
C	1.08127900	2.56252100	-0.53818700
C	-1.12722100	3.53428900	-0.30267100
C	-3.59051700	-0.09294300	-0.97220700
C	-3.68457000	-0.58053900	1.42391400
C	1.62331800	3.84170100	-0.63993400
H	1.72983700	1.68834000	-0.56706000
C	-0.57231700	4.80487000	-0.39081000
H	-2.20266800	3.40820700	-0.18906600
N	-3.08340900	0.52045000	-2.09386800
C	-4.69379600	-0.95754100	-1.12748000
C	-4.76739400	-1.41620400	1.24825300
H	-3.25915900	-0.42490400	2.41332900
C	0.80297500	4.96375800	-0.56274300
H	2.69785700	3.95470200	-0.76595500
H	-1.22215700	5.67542000	-0.33682100
C	-5.26330200	-1.60754800	-0.04928300
H	-5.10447600	-1.08843300	-2.12718600
H	-5.22197500	-1.91973000	2.09723600
H	1.23241600	5.96048600	-0.63443900
H	-6.11540400	-2.26382900	-0.21620500
O	1.68487400	0.71016600	2.44291800
C	2.68330000	-0.02549400	2.35826200
O	2.88378100	-0.87874600	1.39463500
C	3.77131800	-0.00566700	3.39758400
H	4.75796400	0.05632100	2.92773600
H	3.63965500	0.83255800	4.08591600
H	3.74740700	-0.93953400	3.97096500
H	-3.72237400	0.54030700	-2.88017600
H	-2.60213400	1.40230000	-1.97031400

51

18.out

Pd	-0.93228900	1.01595800	-0.22638900
O	1.02118700	3.33715600	0.00466700
C	1.32378200	2.64515700	-0.98703400
O	0.69501600	1.57850400	-1.37496700
C	2.51607100	3.01752900	-1.83006300
H	2.58336800	2.42947800	-2.74901400
H	2.47916800	4.08294600	-2.07887800
H	3.42877100	2.85523700	-1.24394300
C	-0.26688900	1.03287600	2.48129700

C	0.40411800	0.51992900	1.26117700
O	-0.95732300	0.29442500	3.22571200
C	0.80716800	-0.93976200	1.34389000
N	-0.09531500	2.34740100	2.73029900
H	-0.70247900	2.79339200	3.40689600
H	0.28939600	2.92087500	1.98248900
H	1.50932400	-1.07837500	2.17425400
N	1.45451900	-1.43090700	0.13649800
C	0.70415100	-1.74902000	-0.97463600
C	2.86484800	-1.18538500	0.04459200
O	1.19975100	-1.90255300	-2.09251500
C	-0.73315000	-2.01761900	-0.71804800
C	3.39059400	-0.34547700	-0.93835600
C	3.70563900	-1.77849000	0.98798900
C	-1.25298600	-2.10947200	0.57381600
C	-1.59581500	-2.25241700	-1.79214400
C	4.76265800	-0.11354500	-0.97882100
H	2.72761600	0.12699100	-1.65639700
C	5.07459000	-1.53145800	0.94572900
H	3.28580000	-2.43559100	1.74786500
N	-0.35479900	-1.82563300	1.69289800
C	-2.57173900	-2.44232600	0.82373200
C	-2.93187000	-2.56069800	-1.56438100
H	-1.19985300	-2.18182300	-2.80213000
C	5.60741100	-0.70218500	-0.03952000
H	5.16853600	0.54256500	-1.74670800
H	5.72561700	-1.99685600	1.68259800
C	-3.41748400	-2.66554800	-0.26098700
H	-2.93715300	-2.49890300	1.84658000
H	-3.59878900	-2.72709700	-2.40698400
H	6.67815600	-0.51298400	-0.07348600
H	-4.46159300	-2.91203300	-0.08342500
H	1.31041600	1.08917400	1.02758300
O	-2.81340100	1.32483400	-1.44475500
C	-3.46402600	0.90815300	-0.43394400
O	-2.83277000	0.62479800	0.64752000
C	-4.94520500	0.75126200	-0.48810500
H	-5.22990700	0.19115100	-1.38495100
H	-5.32677600	0.24120400	0.39982500
H	-5.41592500	1.73842300	-0.56047800
H	-0.00064000	-2.70066600	2.10068200
H	-0.84946300	-1.28356500	2.45126200

51

19.out

Pd	-0.83311300	1.09840600	-0.22035000
O	1.34384500	3.27248500	0.12568200
C	1.54698000	2.61642200	-0.91452600
O	0.81004200	1.63688700	-1.33891900
C	2.73344500	2.93487700	-1.78575400
H	2.75873700	2.33677600	-2.70006700
H	2.72444100	3.99833100	-2.04685000
H	3.65241800	2.75188800	-1.21669300
C	-0.13072600	1.13929100	2.37891000
C	0.49167600	0.47247100	1.25197500

O	-1.02102100	0.53636100	3.13586500
C	0.69348600	-1.03753500	1.36842800
N	0.17213600	2.38722000	2.68936500
H	-0.40068200	2.88935400	3.35877700
H	0.70261800	2.91516400	1.99413300
H	1.41036600	-1.22390700	2.17617200
N	1.31162900	-1.54339800	0.13017400
C	0.50537900	-1.75386300	-0.96546500
C	2.72488600	-1.36439800	0.00957700
O	0.95571200	-1.89219200	-2.10967400
C	-0.93018500	-1.95774500	-0.66316800
C	3.28203300	-0.55543100	-0.98468200
C	3.55477400	-1.98521000	0.94722000
C	-1.38493600	-2.08113700	0.66009000
C	-1.82467600	-2.18162800	-1.71783300
C	4.66265300	-0.38343400	-1.04017000
H	2.63694500	-0.05805500	-1.70141100
C	4.93253600	-1.79865000	0.89008900
H	3.11729300	-2.61929800	1.71674500
N	-0.52347400	-1.74667000	1.73278800
C	-2.68983900	-2.50323600	0.91621300
C	-3.13753800	-2.54876400	-1.46265100
H	-1.46082600	-2.07668400	-2.73761000
C	5.49237600	-1.00037600	-0.10583000
H	5.08761600	0.24983700	-1.81715900
H	5.56963000	-2.28739200	1.62430600
C	-3.55980600	-2.73384900	-0.14212800
H	-3.02168400	-2.61234500	1.94702900
H	-3.82936300	-2.71090800	-2.28603100
H	6.56992900	-0.85772000	-0.15177800
H	-4.58272700	-3.04284900	0.06389300
H	1.44334700	0.94544000	0.99545500
O	-2.64198400	1.50470100	-1.48039600
C	-3.34512200	1.04591500	-0.52285200
O	-2.76045600	0.69958100	0.56688200
C	-4.82233300	0.91224100	-0.64905400
H	-5.07158300	0.37961300	-1.57272400
H	-5.25036600	0.38374900	0.20623100
H	-5.27610200	1.90751500	-0.71688100
H	-0.32951800	-2.54650500	2.33259500
H	-1.10881400	-0.40706400	2.79580300

36

20.out

C	-1.07952200	2.63779700	-0.54940400
C	-0.13024400	1.67460200	-0.44191000
O	-2.05851400	2.86684500	0.36542500
C	0.09003900	0.80725000	0.75964900
N	-1.14971700	3.55614700	-1.58018700
H	-2.10696800	3.77471400	-1.83847300
H	-0.61602200	3.27215000	-2.39367900
H	0.75680600	1.26281100	1.50377800
N	0.78003200	-0.44767300	0.33571800
C	0.04434000	-1.40037600	-0.32041000
C	2.19739300	-0.38104200	0.20884400

O	0.55979800	-2.35325100	-0.92336400
C	-1.42383600	-1.28493700	-0.16314300
C	2.82298700	-0.50947100	-1.03509800
C	2.96421100	-0.12670100	1.34920900
C	-1.98591700	-0.40511400	0.77694600
C	-2.25682600	-2.16496000	-0.86297700
C	4.20747600	-0.40155600	-1.12655800
H	2.22306700	-0.68789200	-1.92335400
C	4.34731300	-0.00863500	1.24691500
H	2.47211400	-0.02945300	2.31563100
N	-1.15794300	0.52793900	1.45134800
C	-3.35682000	-0.43992800	1.03285700
C	-3.62373300	-2.18341300	-0.62388900
H	-1.80689000	-2.84398300	-1.58416100
C	4.97434500	-0.15120200	0.01062900
H	4.68790600	-0.50286700	-2.09781600
H	4.93598900	0.18718600	2.14088800
C	-4.16901400	-1.32936900	0.33790900
H	-3.77793800	0.24554100	1.76631100
H	-4.26541800	-2.86629100	-1.17588800
H	6.05605000	-0.06441800	-0.06760300
H	-5.23877200	-1.34545800	0.53651700
H	0.60311400	1.59779400	-1.24123900
H	-1.01443100	0.28214000	2.42878400
H	-1.95864100	2.15670200	1.04823300

38

21.out

C	4.50365400	-0.89065500	-0.54767900
C	3.31933800	-1.63024200	-0.57529200
O	4.52927600	0.38963300	-0.63349900
C	2.08389400	-0.87961900	-0.68588900
H	3.29958700	-2.67065400	-0.25948000
N	5.72525700	-1.54563900	-0.33213600
H	6.50690300	-1.00704900	-0.68783500
H	5.74984100	-2.49783100	-0.68006100
C	0.19288400	3.29201000	-0.49013700
C	1.20569700	2.35591700	-0.30826100
C	0.93763100	1.17714700	0.37921200
C	-0.35481400	0.88420900	0.83889300
C	-1.35607400	1.84449600	0.65738900
C	-1.08507700	3.04300600	0.00705100
H	0.40735400	4.22109100	-1.01287200
H	2.21199700	2.53600800	-0.68309900
H	-2.35534400	1.65023000	1.04134500
H	-1.87439500	3.78034900	-0.11620400
C	-0.61418400	-0.37311800	1.59085600
O	0.20752600	-0.79677700	2.42107700
N	1.98919800	0.20246600	0.50767600
N	-1.79428500	-1.02399600	1.40016100
H	2.93056500	0.63374900	0.42139500
H	1.90535300	-0.30847000	1.39268100
H	-1.96508600	-1.75879600	2.08130600
H	2.00757100	-0.20106100	-1.54758600
H	1.16602800	-1.46990800	-0.60760600

C	-2.72686500	-0.92796200	0.33940100
C	-4.07904400	-1.13244800	0.62625400
C	-2.32134500	-0.69310000	-0.97862600
C	-5.02136500	-1.08126600	-0.39627100
H	-4.38342700	-1.32807700	1.65284500
C	-3.27394400	-0.62560300	-1.98989100
H	-1.26531200	-0.57375000	-1.21281700
C	-4.62549200	-0.81713600	-1.70603600
H	-6.07195000	-1.24164100	-0.16291300
H	-2.95069400	-0.43965600	-3.01206300
H	-5.36396000	-0.77102400	-2.50339800

38

22.out

C	-4.51225000	-0.96491300	0.31873400
C	-4.04082300	-0.19871200	1.32941600
O	-4.09013900	-0.86253100	-0.97728500
C	-3.01778700	0.87316900	1.13472900
H	-4.44065200	-0.36316400	2.32560600
N	-5.41936500	-2.00485000	0.45284600
H	-5.98402100	-2.12329700	-0.38221900
H	-6.01631500	-1.89176700	1.26433000
C	0.13537200	3.40093300	-0.32260500
C	-0.90687300	2.59028300	0.10627500
C	-0.86980800	1.19809600	-0.09423000
C	0.28784200	0.63750300	-0.69731900
C	1.32431600	1.47987600	-1.11680200
C	1.25708100	2.85610500	-0.94838900
H	0.06884900	4.47537500	-0.16042900
H	-1.76511400	3.03896900	0.59881000
H	2.19342000	1.03681500	-1.60043600
H	2.06723600	3.49304800	-1.29436900
C	0.35983700	-0.81451700	-0.98180800
O	-0.62182300	-1.45220300	-1.39759800
N	-1.93442900	0.39635900	0.27074600
N	1.56497400	-1.45551000	-0.85380300
H	-3.29299600	-0.28558600	-0.97623800
H	-1.70151300	-0.58009600	0.42067500
H	1.57099900	-2.38028100	-1.27377000
H	-3.44379500	1.76604900	0.64862400
H	-2.63229500	1.21512800	2.10909000
C	2.71988400	-1.11134000	-0.11823900
C	3.95482900	-1.58489900	-0.57277300
C	2.65685700	-0.37382400	1.06968100
C	5.11575000	-1.30680300	0.14206900
H	3.99535500	-2.17103400	-1.48942700
C	3.82575700	-0.08599800	1.76625900
H	1.69539900	-0.03691800	1.44990200
C	5.05988600	-0.54687500	1.30871800
H	6.06983600	-1.68210000	-0.22287400
H	3.76522800	0.49035400	2.68742700
H	5.96861100	-0.32411100	1.86355200

38

22'.out

C	-3.64488200	-0.67645600	0.21762000
C	-3.00833100	0.44036600	-0.21364000
O	-3.36536000	-1.93407700	-0.21429700
C	-2.01420500	0.44152900	-1.31754400
H	-3.26827000	1.38665000	0.25566800
N	-4.72742200	-0.68596500	1.07773100
H	-4.69951300	-1.46113900	1.73234900
H	-4.84904400	0.19428300	1.56501000
C	4.13005100	-1.28559700	0.09238600
C	3.22430400	-2.11609300	0.73359000
C	1.84324300	-2.01616300	0.48720000
C	1.39459600	-1.02223800	-0.41775800
C	2.32989100	-0.19534300	-1.05490600
C	3.69096200	-0.32044400	-0.81818700
H	5.19312900	-1.39827800	0.29843200
H	3.57160000	-2.86928400	1.43969200
H	1.97039800	0.54889500	-1.76370600
H	4.40025100	0.32245200	-1.33340700
C	-0.04895200	-0.90496000	-0.73239000
O	-0.73634500	-1.93754800	-0.91918700
N	0.95837600	-2.80753900	1.19515200
N	-0.58688700	0.33615100	-0.88345600
H	1.37636200	-3.64470500	1.58287500
H	0.09316200	-3.00288500	0.70530800
H	-2.44866100	-1.93143300	-0.59436200
H	-2.17533500	-0.38127300	-2.02095600
H	-2.07346600	1.37169400	-1.89253000
C	-0.04590100	1.48954100	-0.23940600
C	0.09340800	2.68209100	-0.95209000
C	0.28253400	1.44525400	1.11839600
C	0.58305000	3.81727600	-0.31253400
H	-0.16842600	2.71272800	-2.00833800
C	0.78368200	2.58071300	1.74785400
H	0.14391100	0.51743400	1.67247900
C	0.93584100	3.76930200	1.03543500
H	0.69713100	4.74167200	-0.87507100
H	1.04350200	2.53762600	2.80363100
H	1.32269600	4.65736700	1.53066100

8

ACOH.out

O	0.77398100	-1.04365500	0.00017100
C	0.08717400	0.12043800	-0.00063100
O	0.64150400	1.20648900	0.00015100
C	-1.38445400	-0.10980500	-0.00047500
H	-1.67546700	-0.66929400	0.89499800
H	-1.91794600	0.84111400	-0.02634100
H	-1.67152300	-0.71851900	-0.86412000
H	1.72473300	-0.81976900	-0.00047800

3

CO2.out

C	0.00000000	0.00000000	-0.00000000
O	0.00000000	0.00000000	-1.16863500
O	0.00000000	0.00000000	1.16863600

6

H2O.out

O	1.46406300	-0.10751500	0.00344100
H	1.70995500	0.82519100	0.06379600
H	0.48479400	-0.06974400	-0.06449400
O	-1.35818600	-0.00244500	-0.11866700
H	-1.55040700	-0.69038100	0.53687700
H	-1.49136200	0.81462100	0.38563400

4

H2O2.out

O	0.71943000	-0.10254700	-0.06942800
O	-0.71937400	0.10244100	-0.06959300
H	-1.00266500	-0.58801600	0.55641900
H	1.00221800	0.58886000	0.55575200

2

O2.out

O	-0.00000000	0.00000000	0.60808700
O	-0.00000000	0.00000000	-0.60808700

45

Pd3OAc6.out

Pd	0.72987300	-1.60259200	-0.01452200
O	1.81436300	-1.33195100	1.71798800
O	2.37862000	-1.21428700	-1.23182400
C	2.58316000	-0.16335200	-1.91317400
O	2.02793100	0.96747700	-1.72981300
Pd	1.03033100	1.43150200	0.01213600
C	2.58867500	-0.33592100	1.88948800
O	2.58814500	0.73456000	1.20836800
O	-0.20145900	-2.19522600	-1.75401300
O	-0.62839700	-2.60124100	1.20552800
C	-1.55375200	-2.07654900	1.89644000
O	-2.05061700	-0.91621400	1.72893900
Pd	-1.77373400	0.17216100	0.00049300
C	-1.46150900	-2.12602200	-1.91932700
O	-2.27026400	-1.43740800	-1.22468300
O	-1.83174300	1.29593600	-1.72645400
O	-1.93414700	1.84269300	1.23245700
C	-1.13078200	2.34784900	-1.88103900
C	-1.00630100	2.35534700	1.92951600
O	-0.12745700	2.68576300	-1.18199700
O	0.24301900	2.17590800	1.76396100
C	3.61324400	-0.46187800	2.97249400
H	4.49730500	-0.96164300	2.55942100
H	3.91521800	0.51895400	3.34530500
H	3.23529300	-1.07855300	3.79155800
C	-2.14672800	-2.90524000	2.99237800
H	-3.01238500	-3.44547900	2.59149000
H	-1.42767900	-3.63710800	3.36598200
H	-2.49942800	-2.27005900	3.80847100
C	-2.04497600	-2.96389900	-3.01313200
H	-2.92418700	-2.48264200	-3.44725800

H	-1.30225700	-3.16744600	-3.78764200
H	-2.35941100	-3.92319400	-2.58526900
C	-1.55751500	3.28403600	-2.96756100
H	-0.71058200	3.86149400	-3.34402500
H	-2.03594400	2.73726300	-3.78355400
H	-2.29470500	3.98320100	-2.55568200
C	-1.41062600	3.28789700	3.02757200
H	-1.47986000	4.30102500	2.61419800
H	-2.38810200	3.01756600	3.43268900
H	-0.66098400	3.30094100	3.82206600
C	3.59523700	-0.24942500	-3.01176600
H	3.56517800	-1.23061100	-3.49130100
H	3.43926300	0.53886400	-3.75127700
H	4.59296500	-0.11699000	-2.57710800

43

TS6-7.out

Pd	1.04373400	-0.02175400	-0.28265500
O	2.52797700	1.06809400	-1.23070800
C	2.53634800	2.34395300	-0.96633700
O	1.73830800	2.91371300	-0.20489300
O	1.28272800	-2.78434900	1.40584200
C	2.43658300	-2.26527700	1.13888800
O	2.60278900	-1.18654300	0.50839300
C	3.64180200	3.09594000	-1.66031300
H	3.73458300	2.78834700	-2.70621800
H	3.47173700	4.17383600	-1.60601600
H	4.59633100	2.86908100	-1.17135600
C	3.62370400	-3.00763900	1.64133700
H	4.54431700	-2.62999200	1.19446600
H	3.68059200	-2.88749800	2.72929900
H	3.51379100	-4.07656900	1.43828300
C	-0.82549400	-0.19237500	1.55957700
N	-0.50356400	-1.16647900	0.59600900
O	-0.43648900	-0.31599100	2.72259400
N	-0.51047000	1.11122100	-1.08173400
H	-0.13271600	1.87197000	-1.65026100
H	-1.01823200	0.49390900	-1.72550700
C	-1.42101400	1.65922200	-0.09091400
C	-2.08976200	2.84479600	-0.37453100
C	-1.58779400	1.02722000	1.15020600
C	-2.95154200	3.40210800	0.56690100
H	-1.92316500	3.33478200	-1.33231500
C	-2.44370300	1.61075600	2.09021100
C	-3.13409600	2.78114200	1.80013900
H	-3.46999600	4.32965800	0.33556700
H	-2.55928500	1.12382900	3.05623500
H	-3.80169900	3.21577700	2.54006200
C	-1.47932800	-1.61007800	-0.32904200
C	-2.85186000	-1.56632800	-0.04486800
C	-1.04873700	-2.19134900	-1.53195500
C	-3.76819100	-2.08188600	-0.95771100
H	-3.20173900	-1.15058700	0.89863000
C	-1.97218300	-2.70627800	-2.43402000
H	0.02090100	-2.22062000	-1.74512200

C	-3.33797900	-2.65002200	-2.15495700
H	-4.82993000	-2.04212300	-0.72190100
H	-1.62077300	-3.15149000	-3.36277500
H	-4.06014200	-3.05018200	-2.86305300
H	0.45885900	-2.12748200	1.06869300

43

TS6-8.out

Pd	1.05820300	0.01941700	0.10282200
O	1.49600700	3.06041200	-0.80935400
C	2.61412700	2.40812400	-0.78371300
O	2.70040000	1.17027400	-0.56630300
O	2.82868600	-2.10666000	-0.81749500
C	3.02485500	-2.00320700	0.40730300
O	2.39801700	-1.16366400	1.17631800
C	3.84687300	3.20377300	-1.02491700
H	3.93577800	3.97325200	-0.25044600
H	4.73478900	2.57055300	-1.01311400
H	3.77041500	3.72201200	-1.98597800
C	4.05797100	-2.84337000	1.10836800
H	3.73177000	-3.12669100	2.11322400
H	4.28971500	-3.73953000	0.52730100
H	4.97989000	-2.25960000	1.21729700
C	-1.09101300	0.05507400	1.74477100
N	-0.55929600	-1.02556700	0.91854600
O	-0.93715200	-0.00021000	2.95657400
N	-0.28346600	1.24904400	-0.84083500
H	0.64756000	2.34872200	-0.75833300
H	-0.34437000	1.07594600	-1.84652200
C	-1.55410200	1.45863900	-0.30289700
C	-2.52062200	2.17332700	-1.03005400
C	-1.86657600	1.06879200	1.02049800
C	-3.70425500	2.57348100	-0.42847100
H	-2.30224700	2.45074300	-2.06005700
C	-3.04872500	1.52115000	1.62810100
C	-3.96549600	2.27416700	0.91371800
H	-4.42865000	3.14220400	-1.00851100
H	-3.25653600	1.21315000	2.65130200
H	-4.89029700	2.60157800	1.38175500
C	-1.45916400	-1.65116100	-0.04797700
C	-2.79278500	-1.86782800	0.29580000
C	-0.96730000	-2.04495600	-1.28926200
C	-3.64347200	-2.47235800	-0.62519400
H	-3.16291800	-1.56918100	1.27529300
C	-1.82449800	-2.65744000	-2.20015900
H	0.08066300	-1.86930300	-1.53321400
C	-3.16290300	-2.86477300	-1.87320300
H	-4.68579800	-2.63672500	-0.36175000
H	-1.44225200	-2.96536300	-3.17074500
H	-3.83206800	-3.33414000	-2.59089000
H	-0.14861000	-1.72497300	1.54541900

45

TS9.out

Pd	-1.23148900	-0.13075000	0.45506900
----	-------------	-------------	------------

O	-3.12636500	0.41554600	1.12477000
C	-3.79507000	1.17254300	0.30982200
O	-3.37402400	1.57240000	-0.79357700
C	-5.18216100	1.52475600	0.77687100
H	-5.25867900	1.53127300	1.86737500
H	-5.48922100	2.49441600	0.37599900
H	-5.88390100	0.77137600	0.39885600
C	0.65411800	-0.08311200	-1.38946100
N	0.64860700	-0.79729400	-0.18183400
O	0.21672100	-0.53826800	-2.44569700
N	-0.63691900	1.95391100	0.17330500
H	-1.39464600	2.17130400	-0.48482800
H	-0.79607600	2.53550600	0.99653200
C	0.64803200	2.23142700	-0.40345600
C	1.29637700	3.43933400	-0.15300400
C	1.22895500	1.29056200	-1.27031800
C	2.49534000	3.73150600	-0.79547700
H	0.84045100	4.15755200	0.52649900
C	2.41155100	1.61310100	-1.94140300
C	3.04453900	2.82791600	-1.70537900
H	2.99117900	4.67957500	-0.59950700
H	2.84825400	0.88252000	-2.62033000
H	3.97310600	3.06467600	-2.21951100
C	1.71483000	-0.69548200	0.73541900
C	3.03343900	-0.84596100	0.27495300
C	1.48231100	-0.54609700	2.10929200
C	4.09416000	-0.80304000	1.17243300
H	3.21358200	-0.99568100	-0.78932300
C	2.55019200	-0.53040600	3.00195400
H	0.45477300	-0.43951700	2.46082900
C	3.85987000	-0.64755700	2.53906500
H	5.11175200	-0.90521500	0.80007300
H	2.35482700	-0.41356000	4.06617000
H	4.69286600	-0.62317300	3.23812900
O	-1.19577700	-3.28169600	-2.05295900
C	-0.24983000	-3.18241700	-1.26425500
C	-0.43237500	-2.61401900	0.11224200
N	0.99019100	-3.64452500	-1.51448500
C	-1.69578200	-2.20294200	0.56336600
H	0.33153300	-2.86985800	0.84561500
H	1.21292000	-3.96684900	-2.44770800
H	1.76039700	-3.42320200	-0.89611200
H	-2.53878000	-2.33797400	-0.11620000
H	-1.90442100	-2.30785300	1.62911100

45

TS9-10.out

Pd	0.89291700	-0.23310800	-0.36445600
O	2.54216300	0.38578200	-1.47710000
C	3.11188100	1.45030500	-0.99844200
O	2.68226000	2.09947500	-0.02522800
C	4.38896600	1.84471400	-1.68858600
H	4.42800300	1.48812300	-2.72113300
H	4.52222500	2.92962400	-1.66288000
H	5.23029500	1.39426900	-1.14671700

C	-0.87098900	0.17171900	1.54763500
N	-0.75972800	-0.94124400	0.70594200
O	-0.31090300	0.23333800	2.64368300
N	-0.16458100	1.57571500	-0.87853200
H	0.55507600	2.21894100	-0.52833800
H	-0.22535800	1.73162800	-1.88571200
C	-1.42916500	1.85321300	-0.24400000
C	-2.33023800	2.73871200	-0.83016800
C	-1.71592700	1.27853600	1.00508900
C	-3.49679800	3.08891300	-0.15675000
H	-2.09658200	3.17290800	-1.80084200
C	-2.86818000	1.67403200	1.68985700
C	-3.75723800	2.57327800	1.11251900
H	-4.19332900	3.78544900	-0.61784000
H	-3.07900200	1.23167200	2.66218100
H	-4.66102000	2.86025000	1.64490200
C	-1.83608100	-1.37929100	-0.08751000
C	-3.12139300	-1.47159900	0.47465300
C	-1.63929100	-1.82043800	-1.40446600
C	-4.18346100	-1.95226100	-0.28158400
H	-3.27657400	-1.16833100	1.50918000
C	-2.70644500	-2.32145300	-2.14504500
H	-0.64058400	-1.75875800	-1.83964900
C	-3.98528600	-2.38091500	-1.59446000
H	-5.17403400	-2.00352700	0.16686800
H	-2.53382900	-2.65858600	-3.16549400
H	-4.81874300	-2.76349000	-2.17938900
O	2.84401000	-0.82435900	2.35324300
C	3.05907500	-1.26247700	1.21174200
C	2.00650200	-1.93347800	0.40367900
N	4.28020000	-1.20197700	0.62755300
C	0.83735200	-2.35808500	1.04249100
H	2.29933300	-2.42188900	-0.52766200
H	4.97158400	-0.59519300	1.05105400
H	4.36416700	-1.35151500	-0.37008100
H	0.20704300	-3.11496200	0.58516600
H	0.71597800	-2.19553900	2.10992300

45

TS12-13.out

Pd	2.32825000	0.07130000	-0.50787000
O	3.97943000	-0.75248000	0.70711100
C	4.41463400	0.43054300	0.90644700
O	3.81616100	1.41926700	0.35616800
C	5.58328400	0.66610000	1.79945300
H	6.10681200	1.58677900	1.53004600
H	5.22536500	0.77179100	2.83072200
H	6.27344300	-0.18112600	1.77246900
C	0.95735100	-2.41035700	0.08906500
C	1.19283000	-1.56850200	-1.11902400
O	0.54676400	-1.95514900	1.16794500
C	0.43292000	-0.41608400	-1.44588000
H	1.71327400	-2.04565000	-1.95060300
N	1.27802800	-3.70750200	-0.07862900
H	1.11283400	-4.35979700	0.67739000

H	1.54473500	-4.07803600	-0.98099600
H	1.40705000	1.03598100	-1.31978000
H	0.39526500	-0.14567000	-2.50322800
N	-0.73438300	-0.04602900	-0.70560800
C	-1.71772600	-1.01847200	-0.53967400
C	-1.05658300	1.35122600	-0.62148200
O	-1.63522900	-2.11523600	-1.10600400
C	-2.83230200	-0.68098900	0.36877100
C	-2.10374100	1.86766200	-1.38466300
C	-0.32187800	2.18383800	0.22608700
C	-4.15928200	-1.06044300	0.04648300
C	-2.56936600	-0.03777600	1.58803700
C	-2.42204600	3.22028000	-1.29069000
H	-2.66849800	1.20501300	-2.03996200
C	-0.63792400	3.53670100	0.30491500
H	0.48137800	1.75769700	0.82791200
N	-4.47767900	-1.75508800	-1.09912900
C	-5.18044000	-0.72883500	0.95773500
C	-3.58207200	0.25057000	2.48843600
H	-1.53836200	0.21838400	1.82767000
C	-1.68892400	4.05641800	-0.45052100
H	-3.24292800	3.62106100	-1.88149100
H	-0.06978900	4.18312100	0.97052400
H	-3.79194000	-1.74402900	-1.84293600
H	-5.42577600	-1.62170000	-1.42810400
C	-4.89692600	-0.09021900	2.15314400
H	-6.20574700	-0.99545000	0.70466700
H	-3.35645200	0.73483200	3.43511300
H	-1.93790300	5.11319500	-0.38168900
H	-5.71190200	0.14295800	2.83629200

55

TS15-16.out

O	3.16165600	0.54629900	1.26687600
C	4.15022100	1.26725700	0.89970800
O	4.54325200	1.39945000	-0.29972600
C	4.86241700	2.02739200	1.97475200
H	4.87544000	1.46415800	2.91121200
H	5.88117300	2.27825000	1.67054300
H	4.32056700	2.96261500	2.16013700
C	-0.04513700	-2.54168300	-0.95089800
C	0.58448200	-1.34829300	-1.57523500
O	-0.96470400	-2.49686700	-0.12316800
C	0.10543000	-0.02116000	-1.59007000
H	1.29866000	-1.56377700	-2.37000100
N	0.50852800	-3.70616400	-1.35735000
H	0.22712400	-4.56591800	-0.90401300
H	1.32374900	-3.72844500	-1.95594100
H	0.66118900	0.69852100	-2.19322400
N	-1.06714600	0.45777500	-1.07472500
C	-2.27039800	-0.35716400	-1.11068300
C	-1.17510600	1.86545800	-0.85640000
O	-2.44479100	-1.06303900	-2.10114100
C	-3.19321900	-0.22036700	0.00308400
C	-2.33550200	2.54852800	-1.23422500

C	-0.10510700	2.56045400	-0.28558000
C	-4.54503800	-0.65873700	-0.12952300
C	-2.75739200	0.29508800	1.24235700
C	-2.42358400	3.91984700	-1.02473500
H	-3.15751200	2.01235700	-1.70526700
C	-0.20010200	3.93617900	-0.09624900
H	0.79214300	2.02204800	0.02331700
N	-5.05241300	-1.13266500	-1.30266000
C	-5.39965500	-0.52625000	0.98641500
C	-3.60545900	0.39477700	2.32588800
H	-1.71545700	0.58844600	1.34665200
C	-1.35895500	4.61935100	-0.45693700
H	-3.32794500	4.44580000	-1.32252800
H	0.63601800	4.47053800	0.34995400
H	-4.39280600	-1.50997500	-1.97022100
H	-5.94460400	-1.60607800	-1.24671700
C	-4.94068300	-0.01404700	2.18281300
H	-6.43380800	-0.85092400	0.88321400
H	-3.24140100	0.77844600	3.27565200
H	-1.43286200	5.69289300	-0.29869300
H	-5.62548400	0.06130800	3.02571800
O	3.24503700	-0.16273500	-1.69103100
O	4.12343300	-1.32352200	-1.61665400
H	3.60452700	-1.96243900	-2.14289400
Pd	1.85102400	-0.36685100	-0.15100600
O	0.50948000	-0.44908500	1.39387800
C	0.66648600	-1.51000300	2.13153400
O	1.54148400	-2.36882700	1.93524100
C	-0.34167900	-1.63083600	3.24030500
H	-1.26781600	-2.05163500	2.82856300
H	0.02336700	-2.30079600	4.02277900
H	-0.58979500	-0.65564400	3.66982700
H	3.86474900	0.57466900	-1.14079500

51

TS18-19.out

Pd	-0.79433300	1.11020800	-0.23949000
O	1.22166200	3.34209900	0.35129900
C	1.55950700	2.73074900	-0.68109200
O	0.91123500	1.73921500	-1.21029900
C	2.82667900	3.10678900	-1.40377700
H	2.90458700	2.63802400	-2.38818300
H	2.89318000	4.19426400	-1.50723800
H	3.68380900	2.78641300	-0.79876700
C	-0.31481000	0.94839100	2.45552100
C	0.43793600	0.46161500	1.29130700
O	-1.11978700	0.17435800	3.08749500
C	0.74176200	-1.03005500	1.33510800
N	-0.15952200	2.21653500	2.83058000
H	-0.80518200	2.62095300	3.49846700
H	0.34093400	2.83410400	2.19240600
H	1.47419500	-1.21537300	2.12867900
N	1.32391500	-1.52120500	0.08887200
C	0.50337000	-1.75733600	-0.99138200
C	2.73885800	-1.34608300	-0.05382900

O	0.93310000	-1.89487300	-2.14038200
C	-0.92731800	-1.98221900	-0.66453800
C	3.28073500	-0.53616700	-1.05455400
C	3.57989200	-1.97750400	0.86609700
C	-1.37442800	-2.09301400	0.65590100
C	-1.84260100	-2.19850600	-1.70051200
C	4.66113800	-0.37022700	-1.13169200
H	2.62674500	-0.03170800	-1.75794700
C	4.95721500	-1.79656200	0.78691900
H	3.15330800	-2.61452700	1.63917000
N	-0.46347100	-1.79357400	1.73510600
C	-2.68210000	-2.45192600	0.95168400
C	-3.16160100	-2.52764500	-1.41664900
H	-1.49633400	-2.11016500	-2.72751100
C	5.50309100	-0.99464700	-0.21362900
H	5.07621200	0.26503800	-1.91215700
H	5.60409900	-2.29205200	1.50777600
C	-3.57665400	-2.67159600	-0.09145300
H	-2.99816400	-2.53283800	1.98975200
H	-3.86742600	-2.68527400	-2.22887800
H	6.58025500	-0.85566600	-0.27614300
H	-4.60622100	-2.94110700	0.13287500
H	1.37613700	1.00643300	1.15551500
O	-2.54098000	1.57697100	-1.57343200
C	-3.29162800	1.08006600	-0.67298100
O	-2.76589700	0.67619800	0.42608700
C	-4.76272000	0.96823000	-0.87883000
H	-4.96968700	0.48730500	-1.84053700
H	-5.23830400	0.40095700	-0.07499400
H	-5.20477800	1.97035600	-0.91735700
H	-0.19568100	-2.64577400	2.23444900
H	-0.95140400	-0.94705800	2.53337100

38

TS21.out

C	4.50630700	-0.92744200	-0.56954800
C	3.31903200	-1.66799900	-0.41471900
O	4.51888500	0.32120800	-0.82406400
C	2.08864000	-0.95497000	-0.54889300
H	3.33773900	-2.64509500	0.06383600
N	5.73030500	-1.56585000	-0.35406600
H	6.50375700	-1.08429700	-0.79726900
H	5.73537900	-2.55874400	-0.55753800
C	0.21114000	3.27072200	-0.61567000
C	1.21903400	2.35553100	-0.33359000
C	0.93163300	1.21929200	0.41895500
C	-0.38063400	0.94790900	0.83896100
C	-1.37756000	1.88810700	0.55525000
C	-1.08618900	3.04568000	-0.15682100
H	0.44318500	4.16578600	-1.18806400
H	2.23891500	2.51675800	-0.68008800
H	-2.39131700	1.71042300	0.90815200
H	-1.87308300	3.76784800	-0.35977400
C	-0.66616200	-0.26326100	1.65210700
O	0.12620000	-0.64141700	2.53146000

N	1.96972200	0.26009800	0.63524000
N	-1.84290700	-0.92327200	1.46279000
H	2.90352200	0.68011700	0.53799500
H	1.86837100	-0.20522900	1.54142700
H	-2.03693400	-1.61686500	2.17978300
H	1.99746400	-0.29331600	-1.41871300
H	1.16915900	-1.52730100	-0.40065100
C	-2.73070300	-0.90319300	0.36087500
C	-4.09247100	-1.09990200	0.60475600
C	-2.27237600	-0.75218300	-0.95214300
C	-4.99205300	-1.12385900	-0.45652100
H	-4.43761300	-1.23045100	1.62883200
C	-3.18269100	-0.75884100	-2.00373000
H	-1.20811900	-0.63968200	-1.14924700
C	-4.54377900	-0.94299700	-1.76356200
H	-6.05047600	-1.27749100	-0.25627200
H	-2.81848400	-0.63793600	-3.02190300
H	-5.24898500	-0.95524900	-2.59166700

38

TS22.out

C	4.48117600	-0.83745300	-0.48120300
C	3.37328300	-1.55980100	-0.84514100
O	4.40005700	0.42054700	-0.08167100
C	2.05392700	-0.88143100	-0.84376500
H	3.44055100	-2.61648400	-1.08443600
N	5.75796100	-1.40186600	-0.40149100
H	6.47839400	-0.69812000	-0.52250900
H	5.89568100	-2.16120200	-1.05966700
C	0.25704200	3.22103000	-0.46440000
C	1.23407300	2.23549100	-0.37062100
C	0.96077800	1.04581000	0.29956400
C	-0.31196200	0.81006100	0.84123100
C	-1.27917700	1.81809900	0.75045600
C	-0.99653400	3.01891700	0.11101700
H	0.48068400	4.15333400	-0.97781300
H	2.22181000	2.38213100	-0.80413700
H	-2.26003400	1.65536800	1.19311200
H	-1.75644200	3.79475300	0.05712100
C	-0.59570200	-0.45895600	1.56344800
O	0.22216400	-0.93153100	2.37008100
N	1.98983900	0.04592000	0.36194000
N	-1.79807100	-1.06970500	1.37055300
H	3.12920800	0.44948500	0.28627100
H	1.87058200	-0.52608700	1.20269900
H	-1.98390900	-1.81655300	2.03430700
H	1.87551700	-0.20749000	-1.69944100
H	1.20430400	-1.57441600	-0.79590500
C	-2.75040100	-0.90474000	0.33736700
C	-4.09926300	-1.10129400	0.64576900
C	-2.37215800	-0.61177500	-0.97740700
C	-5.06447300	-0.98375200	-0.34936700
H	-4.38299100	-1.34391000	1.66827100
C	-3.34734800	-0.47833500	-1.96033500
H	-1.31994200	-0.50008300	-1.23159100

C -4.69514600 -0.66107600 -1.65378400
H -6.11185600 -1.13844200 -0.09836600
H -3.04486700 -0.24702500 -2.97963400
H -5.45125600 -0.56260800 -2.42954400

38

TS22'.out

C -3.26905300 -1.49193300 -0.34930000
C -2.58848500 -1.09075800 -1.47698200
O -2.64324100 -1.81125200 0.76142900
C -1.11214100 -1.10279500 -1.43693800
H -3.10315300 -0.65987800 -2.33007900
N -4.65730700 -1.61924000 -0.31509700
H -5.03597600 -1.38285700 0.59605300
H -5.12652000 -1.09567800 -1.04604100
C 4.25454500 0.65197600 -1.08182600
C 4.31462700 -0.28552800 -0.07490900
C 3.14221200 -0.88505300 0.44055700
C 1.87840700 -0.47683000 -0.10075200
C 1.86409200 0.48518900 -1.13866100
C 3.02136200 1.04365900 -1.63175900
H 5.17873100 1.08697300 -1.45798100
H 5.27240400 -0.59187000 0.34239900
H 0.91437400 0.78451100 -1.57081900
H 2.98022900 1.77442500 -2.43470600
C 0.66324300 -1.07272700 0.39603400
O 0.58686400 -2.02236000 1.17191100
N 3.25467200 -1.78206400 1.44730300
N -0.64916100 -0.54078200 -0.07041600
H 4.17641500 -2.13233800 1.66990700
H 2.45704200 -2.35785000 1.68010200
H -1.45114100 -1.14504900 0.53755800
H -0.65551700 -2.10504100 -1.42766900
H -0.64184700 -0.53586800 -2.24653600
C -0.89322500 0.86578400 0.21255000
C -1.30586800 1.76613600 -0.76720900
C -0.73766300 1.27528100 1.53654800
C -1.54707300 3.09125700 -0.41233600
H -1.43168500 1.44522000 -1.79814300
C -0.97251400 2.60427100 1.87779100
H -0.43694000 0.55286500 2.29456500
C -1.37967300 3.51464800 0.90498500
H -1.86703200 3.79570000 -1.17702700
H -0.84327000 2.92300900 2.90973900
H -1.56927700 4.55176000 1.17267000

6

(H2O)2.out

O 0 0.2365468955 -2.5368839416 -1.6886446906
H 0 0.6301360150 -2.0443269064 -2.4416900611
H 0 -0.2003285956 -3.2799707999 -2.1257849179
O 0 1.3633726803 -1.0786498400 -3.8292295167
H 0 0.9358961743 -0.2260669251 -3.6552739088
H 0 2.2571518305 -0.9446925871 -3.4785189049

47

14T.out

Pd	0	2.4074728811	-0.7769120477	-0.1872001256
O	0	1.6684433254	0.5951934593	1.7472215602
C	0	2.8816169477	0.6518875512	2.0804901179
O	0	3.7927963828	0.0543654853	1.3959403554
C	0	3.3095758778	1.3992906795	3.3059450507
H	0	4.1136462089	2.1003297517	3.0588486192
H	0	2.4773418023	1.9430963787	3.7584778528
H	0	3.7155520430	0.6949641434	4.0408804849
C	0	0.6577701396	-2.9948911364	-0.2946221848
C	0	1.1395934040	-2.1618837268	-1.4185928338
O	0	0.3799845395	-2.4791755905	0.8093739040
C	0	0.6362848369	-0.9073991888	-1.7367152693
H	0	1.7999097922	-2.6212764123	-2.1521674779
N	0	0.6077437993	-4.3166432814	-0.5115511648
H	0	0.2966002855	-4.9334049504	0.2282600499
H	0	0.7799392179	-4.7090295365	-1.4276622057
H	0	4.8274227061	0.2889567137	-0.1016288042
H	0	1.0676878558	-0.3896790259	-2.5934125704
N	0	-0.4955152310	-0.2958054428	-1.2198035157
C	0	-1.5915215744	-1.0858841972	-0.7338912388
C	0	-0.6458231245	1.1051667672	-1.4503654162
O	0	-1.8195093128	-2.1726079900	-1.2705043556
C	0	-2.3661093852	-0.5401754069	0.3711827638
C	0	-1.8901168491	1.6283864474	-1.8173112658
C	0	0.4631746075	1.9497328831	-1.3501328116
C	0	-3.6979376750	-0.9938622989	0.6086880027
C	0	-1.8016865684	0.4160434448	1.2422415416
C	0	-2.0224932506	2.9917940845	-2.0527095496
H	0	-2.7476056266	0.9676130113	-1.9290821714
C	0	0.3221329370	3.3109362852	-1.6058762457
H	0	1.4317388083	1.5407668861	-1.0605208982
N	0	-4.2913735035	-1.9790928353	-0.1208152493
C	0	-4.4201594766	-0.4036669522	1.6698008425
C	0	-2.5119109184	0.9468454862	2.2989354122
H	0	-0.7715023551	0.7240334802	1.0791190112
C	0	-0.9199187425	3.8395701411	-1.9483823647
H	0	-2.9942073909	3.3897727942	-2.3372669348
H	0	1.1912162089	3.9603928367	-1.5238447391
H	0	-3.8427870764	-2.2808833895	-0.9749750285
H	0	-5.3015080710	-2.0199181653	-0.1002809663
C	0	-3.8411253015	0.5394074827	2.4936044074
H	0	-5.4472361062	-0.7254287674	1.8344223014
H	0	-2.0492763638	1.6697947387	2.9656746939
H	0	-1.0285051562	4.9049024940	-2.1390891973
H	0	-4.4258803880	0.9633355705	3.3081250827
O	0	5.0094347467	0.2829811534	-1.0782348358
O	0	3.8696255134	-0.3021316780	-1.6072338134

17

1a(ACN).out

C	0	-0.3306352551	3.0252265624	-0.0675397726
C	0	0.7328302547	2.4509990374	-0.7484596398
C	0	1.2752064754	1.2532675208	-0.2752453875

C	0	0.7478130494	0.6450143136	0.8740370611
C	0	-0.3258331379	1.2413574160	1.5482339208
C	0	-0.8657793923	2.4272558706	1.0810692105
H	0	-0.7531918625	3.9572471362	-0.4373604396
H	0	1.1468411619	2.9167748679	-1.6399745947
H	0	-0.7169913796	0.7513242561	2.4370623948
H	0	-1.6993637046	2.8924199320	1.6009885796
C	0	1.3233221960	-0.5989872845	1.3504888563
O	0	0.9849332710	-1.2366180391	2.3193150155
O	0	2.3859296672	-1.1105356582	0.5989789193
N	0	2.3341588163	0.6405055382	-0.9193092995
C	0	2.9162622636	-0.5291990571	-0.5285291742
O	0	3.8392096565	-1.0646677987	-1.0964657128
H	0	2.7257959201	1.0726413864	-1.7498569372

17

1a(tol).out

C	0	-0.3325938606	3.0276172373	-0.0657788647
C	0	0.7290820957	2.4529351416	-0.7490689634
C	0	1.2731154769	1.2546167879	-0.2790276026
C	0	0.7474378156	0.6462011737	0.8701924970
C	0	-0.3239295031	1.2417850537	1.5455544242
C	0	-0.8649916414	2.4287961133	1.0818787415
H	0	-0.7547059846	3.9607192542	-0.4336402220
H	0	1.1398064758	2.9228254221	-1.6407518108
H	0	-0.7099070528	0.7468480626	2.4338020233
H	0	-1.6970380513	2.8934158092	1.6046271906
C	0	1.3221291454	-0.6014270192	1.3501829018
O	0	0.9754815890	-1.2323760960	2.3164861804
O	0	2.3891205315	-1.1114554307	0.6019211019
N	0	2.3315200758	0.6373013334	-0.9199684128
C	0	2.9211730606	-0.5350906757	-0.5224691261
O	0	3.8456700853	-1.0555697620	-1.0950008692
H	0	2.7291377424	1.0568835946	-1.7515061890

16

2 (X = NO2).out

C	0	-3.1376134630	0.9768026849	-1.2491337600
C	0	-1.9079970825	0.3660682042	-1.1691254689
C	0	-1.7338094858	-0.8031858135	-0.3894563601
C	0	-2.8484387646	-1.3327659357	0.3050352323
C	0	-4.0774818793	-0.7208373483	0.2254388455
C	0	-4.2282738688	0.4371416299	-0.5516255346
H	0	-3.2730299076	1.8718001743	-1.8484663112
H	0	-1.0554828993	0.7761385440	-1.7061330774
H	0	-2.7207522824	-2.2327732981	0.9025931506
H	0	-4.9329893407	-1.1279153875	0.7552930230
N	0	-0.5162755717	-1.3823220892	-0.2796883233
H	0	-0.4455527938	-2.3100213742	0.1160246165
H	0	0.2178003330	-1.1109312528	-0.9198174716
N	0	-5.4999235585	1.0681600316	-0.6363375823
O	0	-6.4579238981	0.5822650934	-0.0048581398
O	0	-5.6203629168	2.0898067170	-1.3393357586

18

2 (X = OMe).out

C	0	-3.1889376482	0.8913690827	-1.2247033989
C	0	-1.9221986660	0.3296613098	-1.1588828605
C	0	-1.6806539656	-0.8220161407	-0.3919438851
C	0	-2.7588464323	-1.3869359418	0.2985217491
C	0	-4.0349666868	-0.8268988544	0.2380796691
C	0	-4.2562201878	0.3195990120	-0.5256094005
H	0	-3.3681802056	1.7821853911	-1.8238859417
H	0	-1.1004586611	0.7867307048	-1.7093169017
H	0	-2.5978024912	-2.2835835073	0.8963909929
H	0	-4.8456381054	-1.2984597137	0.7873056995
N	0	-0.3870767964	-1.3409422422	-0.2655473447
H	0	-0.3826504412	-2.3341930537	-0.0607738922
H	0	0.1877764823	-1.1610027167	-1.0813656427
O	0	-5.4737574970	0.9505079588	-0.6538594971
C	0	-6.5555407090	0.3764272942	0.0604609868
H	0	-7.4241826552	1.0032183905	-0.1514040990
H	0	-6.7586435171	-0.6508162763	-0.2720016775
H	0	-6.3654722765	0.3702783427	1.1425060343

14

2a(ACN).out

C	0	-3.1548864139	0.1321502455	-1.3276340061
C	0	-1.9023074486	-0.3997758119	-1.6143008353
C	0	-1.3053825451	-1.3300355688	-0.7456747064
C	0	-2.0066995893	-1.7090391142	0.4120863122
C	0	-3.2586933495	-1.1701202678	0.6882061172
C	0	-3.8463122890	-0.2450948251	-0.1756920778
H	0	-3.5971140640	0.8490707534	-2.0186673292
H	0	-1.3700422262	-0.1003242147	-2.5172802895
H	0	-1.5562758990	-2.4324271073	1.0918683039
H	0	-3.7828703988	-1.4825457224	1.5908188761
H	0	-4.8270085224	0.1721929198	0.0435645273
N	0	-0.0251535798	-1.8103278374	-0.9900827547
H	0	0.1710532177	-2.7100713029	-0.5670033048
H	0	0.2434781081	-1.8054881462	-1.9673368330

14

2a(tol).out

C	0	-3.1547275138	0.1309670706	-1.3271283906
C	0	-1.9027920688	-0.4002364080	-1.6126918581
C	0	-1.3075177079	-1.3297357650	-0.7452619237
C	0	-2.0070923301	-1.7082137058	0.4113663150
C	0	-3.2585210105	-1.1700689331	0.6869891906
C	0	-3.8457686397	-0.2472178295	-0.1770736521
H	0	-3.5961147936	0.8488341036	-2.0174226203
H	0	-1.3694889224	-0.0954052100	-2.5133381598
H	0	-1.5564872152	-2.4272375144	1.0958169740
H	0	-3.7821784075	-1.4811469986	1.5901379755
H	0	-4.8264761078	0.1696701139	0.0417616159
N	0	-0.0275544112	-1.8140116554	-0.9931154330
H	0	0.1726646515	-2.7108781303	-0.5690467941
H	0	0.2438394771	-1.8071551380	-1.9681212393

31

5A.out

C	0	1.9207170589	3.1932032988	-0.0167483919
C	0	2.2768268209	2.0559089743	-0.7270594096
C	0	1.8188697928	0.7925883502	-0.3291028016
C	0	0.9624929524	0.7097930301	0.7882408500
C	0	0.6433504436	1.8634921691	1.5189901368
C	0	1.1146415230	3.1043729968	1.1215754329
H	0	2.2910546049	4.1616415692	-0.3467157161
H	0	2.9333993684	2.1267957089	-1.5924734997
H	0	-0.0118768290	1.7636155466	2.3819861017
H	0	0.8484163388	3.9966611240	1.6820799115
C	0	0.3051166134	-0.5304777824	1.1863427411
O	0	-0.0987509423	-0.8621197809	2.2724911540
O	0	2.0016517546	-1.8304725423	0.7054077894
N	0	2.2140307033	-0.3415989766	-1.0341296671
C	0	2.5710537633	-1.5813728308	-0.4032139819
O	0	3.3762591861	-2.2979204390	-1.0230608078
H	0	2.8137753966	-0.1405544708	-1.8281260512
C	0	-3.2146646621	0.9315691444	-1.1286384087
C	0	-1.9341297048	0.3994884549	-1.0077138496
C	0	-1.7556317790	-0.7275601722	-0.2131030170
C	0	-2.8051525116	-1.3245176135	0.4742252879
C	0	-4.0801084487	-0.7812575631	0.3419839622
C	0	-4.2844910932	0.3433388836	-0.4558776545
H	0	-3.3734320340	1.8082583430	-1.7518565255
H	0	-1.0868714593	0.8460733145	-1.5263080474
H	0	-2.6248969711	-2.2009418464	1.0930538420
H	0	-4.9148927098	-1.2410810869	0.8653453491
H	0	-5.2830916975	0.7627153177	-0.5552471087
N	0	-0.4046303981	-1.2505226118	-0.0334163252
H	0	-0.4129721997	-2.2507513918	0.1932080987
H	0	0.1550263895	-1.1313653276	-0.8889911035

37

5B.out

C	0	-1.6315269673	2.6757969260	-1.8358638534
C	0	-0.4447030448	1.9625085514	-1.9125425655
C	0	0.1270419579	1.3906054354	-0.7665664870
C	0	-0.5578334139	1.5217676286	0.4584530687
C	0	-1.7318498044	2.2877797298	0.5284574479
C	0	-2.2742770812	2.8628215074	-0.6091493050
H	0	-2.0503326377	3.1087806993	-2.7420117858
H	0	0.0748681673	1.8563113076	-2.8631783872
H	0	-2.2297418191	2.3801119892	1.4917253295
H	0	-3.1954781783	3.4361980649	-0.5474082166
C	0	-0.1774191781	0.8208035517	1.6817766837
O	0	-0.3385170070	1.1841469657	2.8209555860
O	0	2.0943439035	1.1574037316	1.2624289809
N	0	1.3463119482	0.7333979779	-0.8692851673
C	0	2.4062094428	0.8482077429	0.0811276134
O	0	3.5553210592	0.6042716026	-0.3664387862
H	0	1.6920136341	0.6591950875	-1.8207075704
C	0	-1.5510596025	-2.5561606515	-1.3069638498
C	0	-0.5691434296	-1.9571250506	-0.5208724698
C	0	-0.9451028896	-1.3819753592	0.6871115158

C	0	-2.2652243136	-1.3854713732	1.1264685307
C	0	-3.2345276615	-1.9864843165	0.3302235545
C	0	-2.8787285437	-2.5696867578	-0.8855546201
H	0	-1.2715768653	-3.0138394070	-2.2529892020
H	0	0.4709831817	-1.9380212821	-0.8381868867
H	0	-2.5255046885	-0.9205669603	2.0766682085
H	0	-4.2699712345	-1.9973125684	0.6618240293
H	0	-3.6399904188	-3.0373925125	-1.5058495955
N	0	0.0628399632	-0.7141153601	1.5145714117
H	0	0.0025315049	-1.0612976425	2.4796700901
H	0	1.0343708496	-0.9838917312	1.1951287019
O	0	2.4059683898	-2.0384934560	0.9536444178
H	0	2.6826717746	-2.0350936205	0.0033837263
H	0	1.9644936468	-2.8968099523	1.0532692422
O	0	3.2736704031	-1.8074746289	-1.6776352419
H	0	2.4635629698	-1.7408698838	-2.2051151929
H	0	3.4549215428	-0.8731485454	-1.4164717857

37

5C.out

C	0	-1.9418192555	3.4239278324	-1.1066744886
C	0	-1.1230604998	2.4244072893	-1.6161009763
C	0	-0.4970539204	1.5078296010	-0.7658336983
C	0	-0.7271179512	1.5825941973	0.6213074580
C	0	-1.5040294453	2.6353898526	1.1185170190
C	0	-2.1201577075	3.5462050336	0.2703397863
H	0	-2.4231123106	4.1214851546	-1.7886243320
H	0	-0.9466705649	2.3470348505	-2.6875283000
H	0	-1.6496425290	2.7009631631	2.1951620117
H	0	-2.7404553086	4.3398986503	0.6796266270
C	0	-0.2085511428	0.6190938935	1.6357452687
O	0	0.3646704618	1.0189647873	2.6562322173
O	0	2.0483200543	0.5106827066	0.1378126568
N	0	0.3093977487	0.5209732181	-1.3580516409
C	0	1.5075455290	0.0751184564	-0.8824403743
O	0	2.0130568428	-0.8753306245	-1.6660998284
H	0	0.0646820514	0.2317452572	-2.2986813898
C	0	-1.2693124513	-3.2388776495	-1.1095201248
C	0	-0.5874177472	-2.5505717535	-0.1119475417
C	0	-1.1410894745	-1.3920907258	0.4414551552
C	0	-2.3932115916	-0.9431499119	0.0115264350
C	0	-3.0574192347	-1.6271331591	-1.0022999292
C	0	-2.5009070387	-2.7731139738	-1.5686479523
H	0	-0.8280563983	-4.1362784873	-1.5385439940
H	0	0.3900760553	-2.8882911180	0.2314502335
H	0	-2.8430770529	-0.0654825218	0.4707143886
H	0	-4.0280445064	-1.2679198381	-1.3385534241
H	0	-3.0293123059	-3.3064423961	-2.3558235039
N	0	-0.4194192733	-0.7189399459	1.4507709277
H	0	0.1272492950	-1.3014147505	2.0790194830
H	0	2.5189936312	-0.8165597939	1.3678882642
O	0	2.8864767656	-1.6124230800	1.8076434640
H	0	3.9109794474	-1.8093612861	0.3335353233
H	0	2.2250058875	-2.2937827125	1.6142039419
O	0	4.2687067982	-1.7598747542	-0.5883215871

H 0 4.2792870609 -2.6857707572 -0.8771059580
H 0 2.9009105514 -1.1765440242 -1.2775061177

31

5D(ACN).out

C 0 3.3269223067 2.6847505556 0.6719700600
C 0 3.0037485841 1.7761438491 -0.3272733315
C 0 1.8388872504 1.0068679444 -0.2408527632
C 0 0.9716852483 1.1705743965 0.8606246498
C 0 1.3505021471 2.0491443116 1.8840965792
C 0 2.5070282970 2.8106466721 1.7936314030
H 0 4.2350045760 3.2778273078 0.5852932954
H 0 3.6595907573 1.6373033760 -1.1848589331
H 0 0.6912565529 2.1400222003 2.7449154794
H 0 2.7667135258 3.5035551146 2.5907176892
C 0 -0.3436206573 0.4707489562 1.0490487545
O 0 -0.7176876504 0.1271486744 2.1685141046
O 0 1.3027679883 -1.7825549280 0.0676397758
N 0 1.5591893695 0.0923248855 -1.2827078510
C 0 1.2884997045 -1.2573144583 -1.1751173226
O 0 1.0324482500 -1.9518957351 -2.1367047384
H 0 1.8172523221 0.3754196646 -2.2217942543
C 0 -3.9088190424 -1.2336996053 -1.8612293888
C 0 -2.7283680291 -0.5529384650 -1.5935395432
C 0 -2.2841893487 -0.3934668168 -0.2719625622
C 0 -3.0419873018 -0.9281423285 0.7791970271
C 0 -4.2212567475 -1.6117548159 0.4919428836
C 0 -4.6648629741 -1.7699892463 -0.8189981188
H 0 -4.2361130959 -1.3472221664 -2.8932222946
H 0 -2.1346432823 -0.1396925030 -2.4090631410
H 0 -2.7055017845 -0.8073907207 1.8017026127
H 0 -4.8014957099 -2.0244224843 1.3157938158
H 0 -5.5892724360 -2.3047343170 -1.0277727442
N 0 -1.0806425528 0.3047756200 -0.0922854611
H 0 1.6932452916 -1.1648023567 0.7159923686
H 0 -0.6741445588 0.6709984185 -0.9467470506

31

5D(tol).out

C 0 4.4126881741 0.4850463918 -0.6199568571
C 0 3.5583318593 -0.6099104753 -0.6486155031
C 0 2.2010973924 -0.4677394053 -0.3494140120
C 0 1.6833896468 0.8039583785 -0.0341587799
C 0 2.5736058838 1.8810549646 0.0392202263
C 0 3.9214740835 1.7370825514 -0.2583266330
H 0 5.4659824206 0.3521239531 -0.8590484989
H 0 3.9420253410 -1.6014500366 -0.8857183196
H 0 2.1639783095 2.8479499929 0.3229021380
H 0 4.5852287002 2.5976161766 -0.2120340055
C 0 0.2462643357 1.1377753635 0.2434177344
O 0 -0.0529447374 2.0614456091 0.9919544825
O 0 0.5886132236 -1.3634690746 1.6821634610
N 0 1.3864085118 -1.6313871577 -0.4133620549
C 0 0.6526731350 -2.1838469099 0.6170763436
O 0 0.1181738546 -3.2720398390 0.5471514292
H 0 1.6682026327 -2.3315321058 -1.0888053648

C 0 -4.1279839681 -0.7694622029 -0.8832694779
C 0 -2.7438039276 -0.6858960760 -0.9464622188
C 0 -2.0667797092 0.3803338944 -0.3365744852
C 0 -2.7988242409 1.3630239806 0.3427199561
C 0 -4.1857333950 1.2608699481 0.4001369138
C 0 -4.8601907513 0.2049982763 -0.2076050046
H 0 -4.6346203532 -1.6060839418 -1.3611874054
H 0 -2.1709126700 -1.4577443016 -1.4622461699
H 0 -2.2783778533 2.1858203340 0.8174757854
H 0 -4.7457391656 2.0291704094 0.9309918317
H 0 -5.9451361837 0.1405371513 -0.1553364213
N 0 -0.6697930318 0.3914457465 -0.4541089641
H 0 -0.0001223412 -1.8018816509 2.3212480442
H 0 -0.2889354861 -0.3430243545 -1.0391758099

31

5D.out

C 0 3.7521567039 -0.9088924756 -1.3209721444
C 0 2.4782786900 -0.5955341629 -1.7776560444
C 0 1.3803375565 -0.6296755821 -0.9133738786
C 0 1.5750439059 -0.9561316031 0.4415096409
C 0 2.8551982697 -1.3303046776 0.8661742428
C 0 3.9430222703 -1.2988132886 0.0036205931
H 0 4.5929232179 -0.8687934146 -2.0100343635
H 0 2.3156309842 -0.3298152093 -2.8207206683
H 0 2.9880649960 -1.6096410412 1.9096817468
H 0 4.9330097797 -1.5684156579 0.3634507208
C 0 0.5185673155 -0.9334994099 1.4939349273
O 0 0.3689711138 -1.8921927196 2.2611361115
O 0 -1.1805527844 -1.9023764741 -0.4343765850
N 0 0.1228128507 -0.2929539290 -1.4456957481
C 0 -1.0425466473 -0.9498232974 -1.1897908915
O 0 -2.0496376890 -0.3957323998 -1.9032641882
H 0 0.1155090325 0.3455690810 -2.2335004686
C 0 -1.2994638287 3.3318823319 0.0120379477
C 0 -1.3494575201 2.0897439654 0.6355495200
C 0 -0.1649364037 1.4403085740 0.9976068556
C 0 1.0675085503 2.0570637894 0.7591451614
C 0 1.1065623804 3.2901147391 0.1152716911
C 0 -0.0715547434 3.9321023380 -0.2634796280
H 0 -2.2268383343 3.8270887491 -0.2688864284
H 0 -2.3042218444 1.6048407615 0.8345318400
H 0 1.9885147094 1.5750956835 1.0794380517
H 0 2.0697045292 3.7601850970 -0.0737521319
H 0 -0.0330582875 4.8993503394 -0.7596917805
N 0 -0.2574506355 0.1828543225 1.6322936884
H 0 -1.0577499405 0.0449343893 2.2425344516
H 0 -2.8516231971 -0.9105308183 -1.7005352410

31

5E.out

C 0 3.9320510310 -0.9947149352 -1.3273861559
C 0 2.7192460249 -0.5772058478 -1.8523338815
C 0 1.5648392649 -0.4790340915 -1.0544129737
C 0 1.6753594940 -0.8197040079 0.3167606034
C 0 2.9052333470 -1.2697209031 0.8172976318

C	0	4.0373200969	-1.3453667747	0.0204220983
H	0	4.8034968875	-1.0471796772	-1.9775747574
H	0	2.6393828930	-0.3198986059	-2.9078444466
H	0	2.9546385498	-1.5463152600	1.8692130722
H	0	4.9847726622	-1.6763765437	0.4383606216
C	0	0.5350788050	-0.8530334469	1.2685943269
O	0	0.3420854926	-1.8399180192	1.9927967302
O	0	-1.2235916804	-2.8181687791	-0.6324098975
N	0	0.3576979958	-0.1676670674	-1.6683142584
C	0	-1.9253542659	-1.8891679868	-0.7376601219
O	0	-2.6461810227	-0.9729872574	-0.8340424489
H	0	0.4802569407	0.2455466441	-2.5865033215
C	0	-1.2573417542	3.5184563575	-0.0063218835
C	0	-1.3494452031	2.2121441434	0.4627434866
C	0	-0.1942596671	1.5284985087	0.8606795806
C	0	1.0487256467	2.1686296034	0.8029094837
C	0	1.1295356162	3.4676417863	0.3112246954
C	0	-0.0171242643	4.1479946252	-0.0960083035
H	0	-2.1612746888	4.0411534576	-0.3121309175
H	0	-2.3131277640	1.7082919491	0.5206749400
H	0	1.9424118697	1.6560828377	1.1499250247
H	0	2.1000766494	3.9574861608	0.2656537891
H	0	0.0549598864	5.1661912647	-0.4717546595
N	0	-0.3348402975	0.2048522742	1.3320354941
H	0	-1.1817276069	0.0042877282	1.8572543895
H	0	-0.2956255389	0.3878285130	-1.1273580106

47

TS13-14T.out

Pd	0	2.3463832546	-0.4723684427	-0.2457751150
O	0	1.5852008575	0.3504246206	1.9688379817
C	0	2.7142784557	0.9070937546	1.9959441432
O	0	3.5551012072	0.7503120409	1.0282300012
C	0	3.1136011531	1.7999796957	3.1268731374
H	0	2.5162359364	1.5996328442	4.0196682550
H	0	4.1775257163	1.6921718872	3.3569012803
H	0	2.9469376089	2.8430381449	2.8314994198
C	0	0.6712294616	-2.8223827895	-0.3247566073
C	0	1.2157127818	-1.8959155894	-1.3493735490
O	0	0.2000430715	-2.4179114781	0.7532082716
C	0	0.6865636703	-0.6245048218	-1.6465960185
H	0	1.8479338702	-2.3334196736	-2.1223283632
N	0	0.7728838378	-4.1285158063	-0.6281312700
H	0	0.4500611569	-4.8219854873	0.0343052961
H	0	1.1483942354	-4.4428180937	-1.5127762888
H	0	3.4178866967	-0.4835548901	-1.5035955309
H	0	1.0816247754	-0.1031813065	-2.5199982455
N	0	-0.4834783322	-0.0702322567	-1.1388443781
C	0	-1.5876789060	-0.9176798613	-0.7724896344
C	0	-0.6729962532	1.3335423968	-1.3033382014
O	0	-1.7810862143	-1.9424098234	-1.4307176744
C	0	-2.4050315195	-0.4903944703	0.3517563340
C	0	-1.9130806648	1.8276737882	-1.7226876356
C	0	0.3876421279	2.2161124143	-1.0751380338
C	0	-3.7103746305	-1.0374104738	0.5415941586

C	0	-1.9093224090	0.4368386917	1.2942245291
C	0	-2.0887677514	3.1957390163	-1.8941531248
H	0	-2.7317053910	1.1400815719	-1.9272817772
C	0	0.2052588213	3.5821457929	-1.2696528376
H	0	1.3496083117	1.8315390251	-0.7296022501
N	0	-4.2326895514	-2.0058930390	-0.2561704055
C	0	-4.4783115924	-0.5634550847	1.6296964810
C	0	-2.6622161897	0.8553313817	2.3707422961
H	0	-0.8973694088	0.8139467397	1.1692405580
C	0	-1.0327497237	4.0788539342	-1.6711143640
H	0	-3.0562553837	3.5704386087	-2.2213419712
H	0	1.0359685989	4.2609511432	-1.0884324443
H	0	-3.7496005693	-2.2414670580	-1.1123291329
H	0	-5.2346516769	-2.1389297709	-0.2342855614
C	0	-3.9667347819	0.3566665874	2.5201238151
H	0	-5.4842146733	-0.9596478340	1.7592846022
H	0	-2.2516772725	1.5595186838	3.0895976697
H	0	-1.1749270996	5.1481166228	-1.8107425811
H	0	-4.5837261676	0.6893854031	3.3530450181
O	0	4.3166479531	-0.3801082527	-2.4688336381
O	0	5.2171556023	0.4469715142	-2.1660326145

33

TS1a-5A (X = NO2).out

C	0	3.3389819558	2.7857488842	0.5170033251
C	0	3.2248009060	1.6666493816	-0.2873894130
C	0	2.1245361229	0.7964311598	-0.1895817959
C	0	1.0903148770	1.1416608435	0.7194785931
C	0	1.2563192435	2.2578620825	1.5707873319
C	0	2.3611234919	3.0773381886	1.4754907883
H	0	4.2113831563	3.4276854925	0.4139941672
H	0	4.0134040053	1.4203073683	-0.9956240069
H	0	0.4591904544	2.4822113889	2.2750400173
H	0	2.4580464593	3.9450529889	2.1222346607
C	0	-0.2087184300	0.5126379946	0.8250524964
O	0	-0.9856290127	0.5490740261	1.7442394965
O	0	1.0928237155	-1.8486211010	0.4301854193
N	0	2.1320049316	-0.3437381936	-0.9869988206
C	0	1.9237372641	-1.6999782142	-0.5143618947
O	0	2.5686844674	-2.5673944456	-1.1289105933
H	0	2.9051721810	-0.3345642717	-1.6456618289
C	0	-4.1951403924	0.5860496672	-1.5070615308
C	0	-2.8127866437	0.6405768221	-1.4078784448
C	0	-2.1631183240	-0.2641248907	-0.5754741734
C	0	-2.8497616848	-1.2161555374	0.1716936383
C	0	-4.2316333787	-1.2733814921	0.0761793467
C	0	-4.8789940063	-0.3706387696	-0.7627249976
H	0	-4.7365692280	1.2719513880	-2.1495560963
H	0	-2.2450901930	1.3748029862	-1.9738546552
H	0	-2.3077437902	-1.9070995159	0.8125509752
H	0	-4.8014115713	-2.0046944876	0.6390840662
N	0	-0.7197801814	-0.2037343207	-0.4612031953
H	0	-0.2836936623	-1.1522447592	-0.3364028825
H	0	-0.2925113803	0.2173753607	-1.2955862551
N	0	-6.3328767195	-0.4311528005	-0.8670156246

O 0 -6.9261425027 -1.2960486640 -0.2189687466
O 0 -6.8974876708 0.3854467001 -1.5979517265

35

TS1a-5A (X = OMe).out

C 0 1.4794361846 3.1425495539 -0.0932262359
C 0 2.0376219880 2.0678911594 -0.7723733207
C 0 1.7462952215 0.7557607052 -0.3800032392
C 0 0.8684316847 0.5485998927 0.6982305382
C 0 0.3354395525 1.6410331913 1.3907666938
C 0 0.6354793133 2.9386388396 1.0008988060
H 0 1.7168345413 4.1542442629 -0.4158823325
H 0 2.7142977302 2.2312752401 -1.6091870643
H 0 -0.3422207586 1.4474549087 2.2203187708
H 0 0.2073736874 3.7836593013 1.5339528698
C 0 0.3909166890 -0.7918653830 1.0600665636
O 0 -0.0188746547 -1.1732187997 2.1331461297
O 0 1.9810867493 -1.8596498356 0.6081363366
N 0 2.3164570891 -0.3180700269 -1.0587148041
C 0 2.6494680805 -1.5473982699 -0.4463367884
O 0 3.5313996228 -2.2386968660 -0.9763258335
H 0 2.9570657783 -0.0628439659 -1.8027716794
C 0 -3.1037904486 0.8517511529 -1.2617343833
C 0 -1.8610343675 0.2482637459 -1.1715566788
C 0 -1.7056013353 -0.8754838521 -0.3609182465
C 0 -2.7686617185 -1.3843233161 0.3722878964
C 0 -4.0197467833 -0.7809490497 0.2827779769
C 0 -4.1882496639 0.3414469796 -0.5350357773
H 0 -3.2547057813 1.7236590249 -1.8929562604
H 0 -1.0146851593 0.6437566799 -1.7317019870
H 0 -2.6261525431 -2.2557702827 1.0080026869
H 0 -4.8494102707 -1.1910999491 0.8500609522
N 0 -0.3842625132 -1.4578311121 -0.2052703231
H 0 -0.4317181931 -2.4597443541 0.0052361971
H 0 0.1702211952 -1.3470945480 -1.0619445757
O 0 -5.3668170229 1.0030539294 -0.6911684981
C 0 -6.4855466680 0.5105579635 0.0389061688
H 0 -7.3177820229 1.1688094185 -0.2148637824
H 0 -6.7281738890 -0.5183596254 -0.2541468335
H 0 -6.3014557737 0.5493273265 1.1196786474

31

TS1a-5A.out

C 0 -1.0312301843 -0.0632843957 -1.4930709558
C 0 0.1772412794 -0.3008765989 -0.8526026551
C 0 0.9382335870 0.7656667519 -0.3583254289
C 0 0.4452641100 2.0747764247 -0.5054962048
C 0 -0.7600322810 2.3016722038 -1.1797949550
C 0 -1.5025099782 1.2391837120 -1.6743653917
H 0 -1.6072290116 -0.9072368623 -1.8671469683
H 0 0.5537979844 -1.3156118022 -0.7369262378
H 0 -1.1135733409 3.3263867671 -1.2778292412
H 0 -2.4449249685 1.4202331380 -2.1847792707
C 0 1.0994762796 3.2237110855 0.1276554813
O 0 1.0527972550 4.3876179813 -0.1928271766

O	0	3.0054992899	2.6339201389	-0.0085031319
N	0	2.1555328001	0.5202060899	0.2709459541
C	0	3.2685214337	1.3940640545	0.1995799649
O	0	4.3951811699	0.9040815258	0.3668712317
H	0	2.4280817085	-0.4565823690	0.3046119414
C	0	-2.2653172239	2.6160344962	3.0452117127
C	0	-1.0246368471	2.2974244757	2.5007974331
C	0	-0.0744565736	3.3052515461	2.3688086613
C	0	-0.3357141646	4.6177583891	2.7455048343
C	0	-1.5809177900	4.9213903525	3.2887514522
C	0	-2.5435046434	3.9243397143	3.4381071312
H	0	-3.0149080129	1.8370217938	3.1618201050
H	0	-0.7913323853	1.2808092180	2.1863275146
H	0	0.4275999400	5.3828289325	2.6197686292
H	0	-1.7966538630	5.9420597371	3.5955747875
H	0	-3.5143292077	4.1675237643	3.8640004906
N	0	1.1953468213	2.9926117903	1.7344493941
H	0	1.9445396106	3.6136333018	2.0559067243
H	0	1.4816482068	2.0274876430	1.9372951741

31

TS1a-5D(ACN).out

C	0	3.0074636089	2.9933445283	0.3920205836
C	0	2.9862943594	1.8647743343	-0.4067486935
C	0	2.0030563323	0.8673860277	-0.2511735265
C	0	0.9853877621	1.0934305194	0.7139180687
C	0	1.0604546962	2.2252465511	1.5550567986
C	0	2.0522757041	3.1720831261	1.4015712452
H	0	3.7900645878	3.7354278879	0.2437972121
H	0	3.7587331816	1.7110862807	-1.1587339319
H	0	0.2812471622	2.3539713665	2.3029756175
H	0	2.0790256724	4.0499213460	2.0422006830
C	0	-0.2141940846	0.2974045586	0.8858697522
O	0	-0.9464797333	0.2476570121	1.8387770931
O	0	1.3245791974	-1.8697415816	0.4682725264
N	0	2.0837686843	-0.2702987911	-1.0376857226
C	0	2.0761534922	-1.6640179989	-0.5238638512
O	0	2.7914740327	-2.4297864697	-1.1731430995
H	0	2.8156028554	-0.1911478153	-1.7379769296
C	0	-4.1659373778	0.2195387171	-1.4889490338
C	0	-2.7820714694	0.3053840794	-1.3624350096
C	0	-2.1314412587	-0.5871972488	-0.5186188986
C	0	-2.8218257125	-1.5498156603	0.2087016068
C	0	-4.2057041553	-1.6222604347	0.0757494565
C	0	-4.8765842834	-0.7408444501	-0.7707613957
H	0	-4.6873406346	0.9066090835	-2.1516858479
H	0	-2.2121282465	1.0511556048	-1.9137483267
H	0	-2.2829005067	-2.2329507663	0.8619977374
H	0	-4.7591135555	-2.3727915630	0.6357034178
H	0	-5.9579638517	-0.8040702127	-0.8728603135
N	0	-0.6885372640	-0.4904764385	-0.3709441901
H	0	-0.2130938212	-1.4122991870	-0.2083582598
H	0	-0.2462703738	-0.1039094055	-1.2152907686

31

TS1a-5D(tol).out

C	0	2.8851359082	3.0422930800	0.3838722467
C	0	2.8592422879	1.9433312183	-0.4539946566
C	0	1.9243085498	0.9043428155	-0.2783239003
C	0	0.9605570621	1.0554482770	0.7553684674
C	0	1.0404134887	2.1599398146	1.6305298544
C	0	1.9842878337	3.1493629068	1.4516986308
H	0	3.6310137224	3.8184578159	0.2207448285
H	0	3.5936559433	1.8453774691	-1.2523490782
H	0	0.3079044849	2.2253968988	2.4317808687
H	0	2.0192679080	4.0040732158	2.1223754524
C	0	-0.1779923298	0.1889278429	0.9737497050
O	0	-0.8879721684	0.0964113599	1.9372696002
O	0	1.4541955138	-1.8662294920	0.4705906624
N	0	1.9744022064	-0.2086243818	-1.1000865041
C	0	2.1282409966	-1.6331144433	-0.5614506956
O	0	2.8633060376	-2.3167207165	-1.2625749659
H	0	2.6632187268	-0.0976235881	-1.8391391556
C	0	-4.0159184007	0.2277708305	-1.6005770023
C	0	-2.6369850063	0.2248184443	-1.4159735090
C	0	-2.0843036833	-0.6537411877	-0.4906518575
C	0	-2.8729174161	-1.5153528007	0.2628273588
C	0	-4.2509834276	-1.5001319758	0.0707902872
C	0	-4.8216517429	-0.6326280148	-0.8580886809
H	0	-4.4591039446	0.9057431788	-2.3264338570
H	0	-1.9954686888	0.8958929389	-1.9854805186
H	0	-2.4137759709	-2.1837934581	0.9875046529
H	0	-4.8797284127	-2.1705501471	0.6521904604
H	0	-5.8995397603	-0.6274239648	-1.0048974034
N	0	-0.6492525978	-0.6390884837	-0.2804516624
H	0	-0.2166027111	-1.5660258972	-0.0668084598
H	0	-0.1229594088	-0.3237265558	-1.1103771684

37

TS5B-5C.out

C	0	1.3516758625	3.1346417505	1.4458805118
C	0	1.6758982506	2.4143677716	0.3048972123
C	0	1.4915591158	1.0250636669	0.2492576458
C	0	0.9245555681	0.3789530541	1.3671139568
C	0	0.6559637581	1.1125127637	2.5316756559
C	0	0.8609988038	2.4835754355	2.5792936754
H	0	1.5059178263	4.2118329663	1.4575024648
H	0	2.1032399734	2.9188753571	-0.5603792932
H	0	0.2331730401	0.5865061182	3.3859843478
H	0	0.6255561234	3.0416073591	3.4820430507
C	0	0.4757325351	-1.0232798842	1.3796894893
O	0	0.5892043218	-1.7847632854	2.3212518644
O	0	2.6272417907	-1.5638018753	0.1855294866
N	0	1.8878834402	0.3306998799	-0.8906898979
C	0	2.6659424908	-0.8712796594	-0.8573868163
O	0	3.3031837584	-1.1114293983	-1.9222965969
H	0	2.1597554572	0.9335300730	-1.6604384970
C	0	-2.3344843956	1.0992559260	-1.6897732226
C	0	-1.3720512451	0.1463396166	-1.3619182907
C	0	-1.4103911891	-0.4536363152	-0.1079232966

C	0	-2.3972291131	-0.1166251313	0.8176966648
C	0	-3.3555771924	0.8336942991	0.4807767328
C	0	-3.3240324644	1.4443055783	-0.7725446892
H	0	-2.3076499951	1.5705642420	-2.6697069260
H	0	-0.5934826330	-0.1215703317	-2.0706715921
H	0	-2.4063356757	-0.5962826969	1.7959167212
H	0	-4.1266017462	1.0984674276	1.2008208643
H	0	-4.0725403765	2.1891989839	-1.0336632953
N	0	-0.4013236173	-1.4452651919	0.2664725421
H	0	-0.8791525186	-2.2703947851	0.6436573980
H	0	0.1406682847	-1.9896345927	-0.8182879755
O	0	0.4672051259	-2.6276894894	-1.7829175081
H	0	0.6955669314	-2.0144200610	-2.5646865622
H	0	-0.3289175366	-3.1168071770	-2.0632419033
O	0	1.3299712594	-1.1238601837	-3.7753589301
H	0	0.8962502600	-0.2566771557	-3.7759974805
H	0	2.1626996410	-0.9711384352	-3.2569388014

45

TSRE.out

Pd	0	1.2879685261	0.2245897002	-0.0213598865
O	0	2.5062090301	1.0755237804	-1.5595187747
C	0	3.3166521034	0.2035831736	-2.0367033797
O	0	3.3971999708	-1.0048510504	-1.6908844873
C	0	4.2731189910	0.7062493165	-3.0872107830
H	0	5.1110469936	1.2055425663	-2.5865758080
H	0	4.6741634334	-0.1131330004	-3.6875607060
H	0	3.7908114437	1.4431752524	-3.7348957835
C	0	-1.1482893175	0.4751068009	1.8264888065
N	0	-0.9557520807	-0.8277263550	1.4008497468
O	0	-0.4014253098	0.9756227173	2.6752454519
N	0	0.1302527287	2.2228421881	0.1904301665
H	0	0.4293229171	2.5149745434	1.1208941292
H	0	0.4938611263	2.9038114965	-0.4741113749
C	0	-1.2982381524	2.1844923885	0.1215642465
C	0	-1.9877517228	2.9385752461	-0.8283159371
C	0	-2.0225195515	1.3297044821	0.9798352699
C	0	-3.3756854599	2.8723186090	-0.9073100641
H	0	-1.4263531854	3.5876517881	-1.4990552699
C	0	-3.4133194868	1.2825173719	0.9009572527
C	0	-4.0934630757	2.0582205252	-0.0333068927
H	0	-3.8975638591	3.4724665624	-1.6496481862
H	0	-3.9613527506	0.6275944911	1.5747948882
H	0	-5.1789662202	2.0179189413	-0.0842598656
C	0	-1.8678813097	-1.4469222161	0.4845371807
C	0	-3.0710363802	-1.9497149693	0.9796435449
C	0	-1.5766317521	-1.5355796142	-0.8783899428
C	0	-3.9923627700	-2.5241301017	0.1073154058
H	0	-3.2820128610	-1.8754935890	2.0448705757
C	0	-2.4993431197	-2.1173901569	-1.7430381793
H	0	-0.6404082070	-1.1227757561	-1.2574405171
C	0	-3.7088041538	-2.6099017461	-1.2540954308
H	0	-4.9331286768	-2.9079309303	0.4962688161
H	0	-2.2749180179	-2.1757227565	-2.8062080935
H	0	-4.4288038647	-3.0598139252	-1.9343904572

O	0	3.6989164730	-1.2785724629	1.5224663650
C	0	3.0622491467	-2.0403596893	0.7785723689
C	0	1.9146729387	-1.5463083808	-0.0500475877
N	0	3.3228786608	-3.3566720054	0.6758247657
C	0	0.4133238959	-1.3015449807	1.4498162667
H	0	1.4838711675	-2.2879655982	-0.7350510660
H	0	4.0983364488	-3.7565766349	1.1902456328
H	0	2.8338556258	-3.9456175393	0.0151800759
H	0	0.4122458096	-2.3936136391	1.3829228823
H	0	0.8976558540	-0.9936968435	2.3762896350

MECP

Energy of triplet state of MECP: -1440.7691985700

Energy of singlet state of MECP: -1440.7692048000

46	2.0911178	-0.5346060	-0.0876352
8	1.2964657	0.7452923	1.8719741
6	2.4942966	0.7723790	2.2611574
8	3.4332394	0.2215737	1.5751626
6	2.8672400	1.4273692	3.5556736
1	3.6610839	2.1634603	3.3903158
1	2.0088669	1.9156855	4.0226125
1	3.2687436	0.6761055	4.2453697
6	0.3863357	-2.7618250	-0.4104376
6	0.8778142	-1.8317913	-1.4514468
8	0.0638071	-2.3434451	0.7223370
6	0.3582955	-0.5645563	-1.6849289
1	1.5626869	-2.2206389	-2.2033716
7	0.3800528	-4.0633876	-0.7309847
1	0.0696214	-4.7436096	-0.0487960
1	0.5822699	-4.3770566	-1.6711018
1	4.4677758	0.5934703	0.1092666
1	0.8024405	0.0260618	-2.4860945
7	-0.7987061	-0.0163832	-1.1547086
6	-1.8878336	-0.8649767	-0.7585217
6	-0.9773992	1.3939281	-1.2863786
8	-2.0803606	-1.9095719	-1.3849772
6	-2.6967787	-0.4228366	0.3675220
6	-2.2253812	1.9152603	-1.6439097
6	0.1086071	2.2531012	-1.0980758
6	-4.0231538	-0.9197734	0.5392307
6	-2.1715462	0.4749320	1.3211380
6	-2.3843940	3.2892518	-1.7839843
1	-3.0650202	1.2464680	-1.8236054
6	-0.0590871	3.6258534	-1.2581734
1	1.0801445	1.8472483	-0.8141908
7	-4.5776657	-1.8587271	-0.2761555
6	-4.7815069	-0.4254510	1.6236492
6	-2.9164445	0.9109148	2.3971620
1	-1.1441757	0.8127404	1.2070538
6	-1.3047792	4.1511559	-1.5920562
1	-3.3583776	3.6856735	-2.0627895
1	0.7925495	4.2862655	-1.1079030
1	-4.1017942	-2.0878204	-1.1381833
1	-5.5866678	-1.9242869	-0.2822318
6	-4.2412637	0.4650392	2.5285955

1	-5.8047399	-0.7788829	1.7389176
1	-2.4844931	1.5901258	3.1272085
1	-1.4334794	5.2247402	-1.7090826
1	-4.8534581	0.8164842	3.3574010
8	4.6855345	0.6272363	-0.8598671
8	3.5860880	0.0225422	-1.4471259

9. References

- (1) M. J. Frisch, G. W. T., H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc. Gaussian 16, Revision C.01. Wallingford CT 2016.
- (2) Zhao, Y.; Truhlar, D. G. A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. *J. Chem. Phys.* **2006**, *125*, 194101
- (3) (a) Yamout, L. S.; Ataya, M.; Hasanayn, F.; Holland, P. L.; Miller, A. J.; Goldman, A. S. Understanding terminal versus bridging end-on N₂ coordination in transition metal complexes. *J. Am. Chem. Soc.* **2021**, *143*, 9744–9757. (b) Raju, R. K.; Bengali, A. A.; Brothers, E. N. A unified set of experimental organometallic data used to evaluate modern theoretical methods. *Dalton Trans.* **2016**, *45*, 13766–13778. (c) Gusev, D. G. Assessing the accuracy of M06-L organometallic thermochemistry. *Organometallics* **2013**, *32*, 4239–4243. (d) Minenkov, Y.; Singstad, Å.; Occhipinti, G.; Jensen, V. R. The accuracy of DFT-optimized geometries of functional transition metal compounds: A validation study of catalysts for olefin metathesis and other reactions in the homogeneous phase. *Dalton Trans.* **2012**, *41*, 5526–5541. (e) Zhao, Y.; Truhlar, D. G. Density functionals with broad applicability in chemistry. *Acc. Chem. Res.* **2008**, *41*, 157–167.
- (4) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions. *J. Phys. Chem. B* **2009**, *113*, 6378–6396.
- (5) (a) Bergner, A.; Dolg, M.; Küchle, W.; Stoll, H.; Preuß, H. Ab Initio energy-adjusted pseudopotentials for elements of groups 13 – 17. *Mol. Phys.* **1993**, *80*, 1431 – 1441. (b) Dolg, M.; Wedig, U.; Stoll, H.; Preuss, H. Energy - adjusted ab initio pseudopotentials for the first row transition elements. *J. Chem. Phys.* **1987**, *86*, 866 – 872. (c) Hariharan, P. C.; Pople, J. A. The influence of polarization functions on molecular orbital hydrogenation energies. *Theor. Chim. Acta* **1973**, *28*, 213–222.
- (6) Fukui, K. The path of chemical reactions-the IRC approach. *Acc. Chem. Res.* 1981, *14*, 363–368.
- (7) Harvey, JN.; Aschi, M.; Schwarz, H.; Koch, W. The singlet and triplet states of phenyl cation. A hybrid approach for locating minimum energy crossing points between non-interacting potential energy surfaces. *Theor. Chem. Acc.* **1998**, *99*, 95-99.