

Reaction of *N*-Vinyllic Phosphazenes with α,β -
unsaturated Aldehydes. Azatriene-Mediated
Synthesis of Dihydropyridines and Pyridines
Derived from β -Amino Acids.

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CONTENTS of the Supporting Information:

General Experimental Remarks.....	S3
λ^5 -phosphazenes	S3
Pyridines 7	S5
Azatrienes 11	S5
Pyridines 7 and 7'	S9
Table 1 including the total energies (hartree) and ZPVE.....	S12
Tables including the Cartesian Coordinates (\AA).....	S16
Computational Methods.....	S74
References.....	S75

General Methods. All solvents used in reactions were freshly distilled from appropriate drying agents before use. All other reagents were recrystallized or distilled as necessary. All reactions were performed under an atmosphere of dry nitrogen. ^1H (300 MHz), ^{13}C (75 MHz) and ^{31}P NMR (120 MHz) spectra were recorded on a 400 MHz spectrometer using CDCl_3 solutions with TMS as an internal reference ($\delta = 0.00$ ppm) for ^1H and ^{13}C NMR spectra, and phosphoric acid (85%) ($\delta = 0.00$ ppm) for ^{31}P NMR spectra. Chemical shifts (δ) are reported in ppm. Coupling constants (J) are reported in Hz. Phosphazenes **6a**, **c**, **e**¹ were synthesized according to literature procedures.

4-(Ethoxycarbonyl)-1,1,1-trimethyl-2-aza-1- λ^5 -phosphabuta-1,3-diene (6b). A solution of 0.705 g (5 mmol) of ethyl 3-azidoacrylate in anhydrous CH_2Cl_2 (3 mL) was added dropwise to a 0 °C solution of 5 mL (5 mmol) of trimethylphosphine (hexane 1M) in anhydrous CH_2Cl_2 (8 mL), and the mixture was stirred for 30 minutes at 0 °C. Phosphazene **6b** is unstable during distillation and/or chromatography and were used without purification for the following reactions. It was obtained a 85:15 diastereomeric mixture of *E/Z* isomers of **6b**. ^1H NMR (300 MHz, CDCl_3) of crude reaction mixture δ 1.14-1.22 (m, 6H), 1.61 (d, $^2J_{\text{(P,H)}} = 12.8$ Hz, 9H,) for isomer *E*, 1.81 (d, $^2J_{\text{(P,H)}} = 12.8$ Hz, 9H) for isomer *Z*, 3.98-4.09 (m, 8H), 4.59 (dd, $^3J_{\text{(H,H)}} = 7.6$ Hz, $^4J_{\text{(P,H)}} = 3.1$ Hz, 1H) for isomer *Z*, 4.99 (d, $^3J_{\text{(H,H)}} = 12.4$ Hz, 1H) for isomer *E*, 6.97 (dd, $^3J_{\text{(H,H)}} = 7.6$ Hz, $^3J_{\text{(H,H)}} = 35.5$ Hz, 1H) for isomer *Z*, 7.86 (dd, $^3J_{\text{(H,H)}} = 12.4$ Hz, $^3J_{\text{(P,H)}} = 33.3$ Hz, 1H) for isomer *E* ppm; ^{13}C NMR (75 MHz, CDCl_3) of crude reaction mixture δ 13.4 (d, $^2J_{\text{(P,C)}} = 66$ Hz) for isomer *Z*, 13.5 (d, $^2J_{\text{(P,C)}} = 66$ Hz) for isomer *E*, 14.3 for isomer *E*, 14.5 for isomer *Z*, 56.7 for isomer *E*, 57.2 for isomer *Z*, 92.2 (d, $^3J_{\text{(P,C)}} = 27$ Hz) for isomer *E*, 95.5 (d, $^3J_{\text{(P,C)}} = 29$ Hz) for isomer *Z*, 153.7 (d, $^2J_{\text{(P,C)}} = 5$ Hz) for isomer *Z*, 156.2 (d, $^2J_{\text{(P,C)}} = 4$ Hz) for isomer *E*, 166.1 for isomer *E*, 169.4 for isomer *Z* ppm; ^{31}P NMR (CDCl_3 , 120 MHz) δ 27.41 for isomer *Z*, 28.12 for isomer *E* ppm.

4-(Ethoxycarbonyl)-3-phenyl-1,1,1-trimethyl-2-aza-1- λ^5 -phosphabuta-1,3-diene

(6d). A solution of 1.086 g (5 mmol) of ethyl 3-azido-3-phenylacrylate in anhydrous CH_2Cl_2 (3 mL) was added dropwise to a 0 °C solution of 5 mL (5 mmol) of trimethylphosphine (hexane 1M) in anhydrous CH_2Cl_2 (8 mL), and the mixture was stirred for 30 minutes at 0 °C. Phosphazene **6d** is unstable during distillation and/or chromatography and were used without purification for the following reactions. It was obtained a 15:85 diastereomeric mixture of *E/Z* isomers of **6d**. ^1H NMR (300 MHz, CDCl_3) of crude reaction mixture δ 0.99 (t, $^3J_{(\text{H,H})} = 7.2$ Hz, 3H) for isomer *E*, 1.20 (t, $^3J_{(\text{H,H})} = 7.2$ Hz, 3H) for isomer *Z*, 1.44 (d, $^2J_{(\text{P,H})} = 12.8$ Hz, 9H) for isomer *E*, 1.65 (d, $^2J_{(\text{P,H})} = 12.5$ Hz, 9H) for isomer *Z*, 3.85 (q, $^3J_{(\text{H,H})} = 7.2$ Hz, 2H) for isomer *E*, 4.04 (q, $^3J_{(\text{H,H})} = 7.2$ Hz, 2H) for isomer *Z*, 4.90 (d, $^4J_{(\text{P,H})} = 0.9$ Hz, 1H) for isomer *E*, 5.36 (d, $^4J_{(\text{P,H})} = 1.2$ Hz, 1H) for isomer *Z*, 7.20-7.64 (m, 10H) ppm; ^{13}C NMR (75 MHz, CDCl_3) of crude reaction mixture δ 14.3 for isomer *E*, 14.7 for isomer *Z*, 17.9 (d, $^2J_{(\text{P,C})} = 70$ Hz) for isomer *E*, 18.1 (d, $^2J_{(\text{P,C})} = 71$ Hz) for isomer *Z*, 57.9 for isomer *Z*, 60.1 for isomer *E*, 91.3 (d, $^3J_{(\text{P,C})} = 17$ Hz) for isomer *Z*, 95.2 (d, $^3J_{(\text{P,C})} = 20$ Hz) for isomer *E*, 126.0-132.8, 143.5 (d, $^2J_{(\text{P,C})} = 22$ Hz) for isomer *E*, 144.6 (d, $^2J_{(\text{P,C})} = 21$ Hz) for isomer *Z*, 164.4 for isomer *Z*, 165.1 for isomer *E* ppm; ^{31}P NMR (CDCl_3 , 120 MHz) δ 14.81 for isomer *Z*, 15.60 for isomer *E* ppm.

1,1,1,1-Tetramethyl-4-(methoxycarbonyl)-2-aza-1 λ^5 -phosphabuta-1,3-diene (6k).

A solution of 0.705 g (5 mmol) of methyl 3-azidocrotonate in anhydrous CH_2Cl_2 (3 mL) was added dropwise to a 0 °C solution of 5 mL (5 mmol) of trimethylphosphine (hexane 1M) in anhydrous CH_2Cl_2 (8 mL), and the mixture was stirred for 30 minutes at 0 °C. Phosphazene **6f** is unstable during distillation and/or chromatography and were used without purification for the following reactions. It was obtained the *Z* isomer of **6f**. ^1H NMR (300 MHz, CDCl_3) of crude reaction mixture δ 1.63 (d, $^2J_{(\text{P,H})} = 12.7$ Hz, 9H),

2.28 (s, 3H), 3.54 (s, 3H), 4.48 (s, 1H) ppm; ^{13}C NMR (75 MHz, CDCl_3) of crude reaction mixture δ 12.9 (d, $^2J_{\text{P,C}} = 70$ Hz), 23.4 (d, $^3J_{\text{P,C}} = 24$ Hz), 47.8, 90.1 (d, $^3J_{\text{P,C}} = 18$ Hz), 167.1, 169.1 (d, $^4J_{\text{P,C}} = 8$ Hz) ppm; ^{31}P NMR (CDCl_3 , 120 MHz) δ 27.41 ppm.

Ethyl 3-pyridinecarboxylate (7a). The general procedure was followed using acrolein **2a** (0.201 mL, 3 mmol). The crude oil was chromatographed on silica gel (10:1 hexane/AcOEt) to give 0.127 g (28%) of **7a** as a yellow oil ($R_f = 0.45$, hexane/AcOEt 2:1) (See the spectroscopy data for the ethyl nicotinate).²

Ethyl 6-phenyl-3-pyridinecarboxylate (7b). The general procedure was followed using cinnamaldehyde **2b** (0.378 mL, 3 mmol). The crude oil was chromatographed on silica gel (20:1 hexane/AcOEt) to give 0.218 g (32%) of **7b** as a yellow oil ($R_f = 0.52$, hexane/AcOEt 2:1): ^1H NMR (300 MHz, CDCl_3) δ 1.34 (t, $^3J_{\text{H,H}} = 7.2$ Hz, 3H), 4.35 (q, $^3J_{\text{H,H}} = 7.2$ Hz, 2H), 7.19-7.29 (m, 3H), 7.71 (d, $^3J_{\text{H,H}} = 8.3$ Hz, 1H), 7.98 (d, $^3J_{\text{H,H}} = 7.8$ Hz, 2H), 8.25 (dd, $^5J_{\text{H,H}} = 2.1$ Hz, $^3J_{\text{H,H}} = 8.3$ Hz, 1H), 9.21 (d, $^5J_{\text{H,H}} = 2.1$ Hz, 1H) ppm; ^{13}C NMR (75 MHz, CDCl_3) δ 14.2, 61.2, 119.6, 124.4, 127.2, 128.8, 129.8, 137.7, 138.2, 150.9, 160.7, 165.3 ppm; IR (NaCl) 1713; M/S (EI) m/z 227 (M^+ , 84). Anal. Calcd. for $\text{C}_{14}\text{H}_{13}\text{NO}_2$: C, 74.08; H, 5.77; N, 6.17. Found, C, 74.10; H, 5.78; N, 6.16.

Ethyl 5-methyl-3-pyridinecarboxylate (7c). The general procedure was followed using methacrolein **2c** (0.246 mL, 3 mmol). The crude oil was chromatographed on silica gel (10:1 hexane/AcOEt) to give 0.149 g (30%) of **7c** as a yellow oil ($R_f = 0.36$, hexane/AcOEt 2:1); ^1H NMR (300 MHz, CDCl_3) δ 1.33 (t, $^3J_{\text{H,H}} = 7.2$ Hz, 3H), 2.32 (s, 3H), 4.33 (q, $^3J_{\text{H,H}} = 7.2$ Hz, 2H), 8.03 (s, 1H), 8.53 (s, 1H) ppm; ^{13}C NMR (75 MHz, CDCl_3) δ 14.1, 18.1, 61.2, 126.1, 132.9, 137.2, 147.9, 153.7, 165.4 ppm; IR

(NaCl) 1715; M/S (EI) m/z 165 (M^+ , 69). Anal. Calcd. for $C_9H_{11}NO_2$: C, 65.44; H, 6.71; N, 8.48. Found: C, 65.66; H, 6.73; N, 8.47.

Ethyl 2-phenyl-4-methyl-3-pyridinecarboxylate (8). Crotonaldehyde **2d** (0.065 mL, 0.80 mmol) was added to a 0-10 °C solution of ethyl 2-amino-2-phenyl-prop-2-enoate **9** (0.15 g, 0.80 mmol), in anhydrous toluene (10 mL) under N_2 , and the mixture was stirred at 110 °C for 8 days. Evaporation of solvent under reduced pressure afforded an oil that was chromatographed on silica gel (20:1 hexane/AcOEt) to give 0.15g (83%) of **8** as a yellow oil (R_f = 0.26, hexane/AcOEt 2:1); 1H NMR (300 MHz, $CDCl_3$) δ 0.95 (t, $^3J_{HH} = 7.2$ Hz, 3H), 2.36 (s, 3H), 4.06 (q, $^3J_{HH} = 7.2$ Hz, 2H), 7.06 (d, $^3J_{HH} = 5$ Hz, 1H), 7.34-7.53 (m, 5H) 8.5 (d, $^3J_{HH} = 5$ Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 13.6, 19.4, 61.4, 123.6, 129.2, 128.2, 128.6, 140.1, 145.5, 149.6, 156.7, 168.6 ppm; IR (NaCl) 1723, 1567; M/S (EI) m/z 241 (M^+ , 13)

1-(Ethoxycarbonyl)-3-azahexa-1,3,5-triene (11a). The general procedure A was followed using phosphazene **6a** (1.252 g, 4 mmol) and acrolein **2a** (0.268 mL, 4 mmol) (room temperature/1 h). 1H NMR (300 MHz, $CDCl_3$) of crude reaction mixture (**11a** + Ph_2MePO) δ 1.16 (t, $^3J_{(H,H)} = 7.2$ Hz, 3H), 1.96 (d, $^2J_{(P,H)} = 13.0$ Hz, 3H), 4.08 (q, $^3J_{(H,H)} = 7.2$ Hz, 2H), 5.84 (d, $^3J_{(H,H)} = 17.1$ Hz, 1H), 5.90 (d, $^3J_{(H,H)} = 9.9$ Hz, 1H), 5.97 (d, $^3J_{(H,H)} = 13.2$ Hz, 1H), 6.36-6.05 (m, 1H), 7.31-7.69 (m, 11H), 7.93 (d, $^3J_{(H,H)} = 9.0$ Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) of crude reaction mixture (**11a** + Ph_2MePO) δ 13.8, 16.5 (d, $^1J_{(P,C)} = 74$ Hz), 59.9, 118.8, 128.4-131.4, 132.0, 132.8, 134.2, 136.1, 154.6, 166.0, 169.3 ppm. The general procedure B was followed using phosphazene **6b** (4 mmol), prepared “in situ”, and 0.268 mL (4 mmol) of acrolein **2a** (room temperature/0.5 h). 1H NMR (300 MHz, $CDCl_3$) of crude reaction mixture (**11a** + Me_3PO) δ 1.16 (t, $^3J_{(H,H)} = 7.2$ Hz, 3H), 1.47 (d, $^2J_{(P,H)} = 12.8$ Hz, 9H), 4.08 (q, $^3J_{(H,H)} = 7.2$ Hz, 2H), 5.84

(d, $^3J_{(H,H)} = 17.1$ Hz, 1H), 5.90 (d, $^3J_{(H,H)} = 9.9$ Hz, 1H), 5.97 (d, $^3J_{(H,H)} = 13.2$ Hz, 1H), 6.21 (ddd, $^3J_{(H,H)} = 9.0$ Hz, $^3J_{(H,H)} = 9.9$ Hz, $^3J_{(H,H)} = 17.1$ Hz, 1H), 7.71 (d, $^3J_{(H,H)} = 13.2$ Hz, 1H), 7.93 (d, $^3J_{(H,H)} = 9.0$ Hz, 1H) ppm; ^{13}C NMR (75 MHz, CDCl_3) δ 13.8, 17.8 (d, $^1J_{(P,C)} = 70$ Hz, 59.9, 118.8, 132.0, 136.1, 154.6, 166.0, 169.3 ppm).

1-(Ethoxycarbonyl)-6-phenyl-3-azahexa-1,3,5-triene (11b). The general procedure A was followed using phosphazene **6a** (1.252 g, 4 mmol) and cinnamaldehyde **2b** (0.504 mL, 4 mmol) (room temperature/7 h). ^1H NMR (300 MHz, CDCl_3) of crude reaction mixture (**11b** + Ph_2MePO) δ 1.25 (t, $^3J_{(H,H)} = 7.2$ Hz, 3H), 1.96 (d, $^2J_{(P,H)} = 13.0$ Hz, 3H), 4.17 (q, $^3J_{(H,H)} = 7.2$ Hz, 2H), 6.08 (d, $^3J_{(H,H)} = 13.1$ Hz, 1H), 6.98 (dd, $^3J_{(H,H)} = 9.0$ Hz, $^3J_{(H,H)} = 16.0$ Hz, 1H), 7.14 (d, $^3J_{(H,H)} = 15.9$ Hz, 1H), 7.31-7.70 (m, 15H), 7.77 (d, $^3J_{(H,H)} = 13.1$ Hz, 1H), 8.14 (d, $^3J_{(H,H)} = 9.0$ Hz, 1H) ppm; ^{13}C NMR (75 MHz, CDCl_3) of crude reaction mixture (**11b** + Ph_2MePO) δ 14.2, 16.5 (d, $^1J_{(P,C)} = 74$ Hz), 60.3, 118.6, 126.3-131.7, 147.1, 152.6, 155.5, 167.5, 169.4 ppm. The general procedure B was followed using phosphazene **6b** (4 mmol), prepared “in situ”, and 0.504 mL (4 mmol) of cinnamaldehyde **2c** (room temperature/1 h). ^1H NMR (300 MHz, CDCl_3) of crude reaction mixture (**11b** + Me_3PO) δ 1.25 (t, $^3J_{(H,H)} = 7.2$ Hz, 3H), 1.47 (d, $^2J_{(P,H)} = 12.8$ Hz, 9H), 4.17 (q, $^3J_{(H,H)} = 7.2$ Hz, 2H), 6.08 (d, $^3J_{(H,H)} = 13.1$ Hz, 1H), 6.98 (dd, $^3J_{(H,H)} = 9.0$ Hz, $^3J_{(H,H)} = 16.0$ Hz, 1H), 7.14 (d, $^3J_{(H,H)} = 15.9$ Hz, 1H), 7.30-7.51 (m, 5H), 7.77 (d, $^3J_{(H,H)} = 13.1$ Hz, 1H), 8.14 (d, $^3J_{(H,H)} = 9.0$ Hz, 1H) ppm; ^{13}C NMR (75 MHz, CDCl_3) of crude reaction mixture (**11b** + Me_3PO) δ 14.2, 17.8 (d, $^1J_{(P,C)} = 70$ Hz), 60.3, 118.6, 126.3-131.7, 147.1, 152.6, 155.5, 167.5, 169.4 ppm

1-(Ethoxycarbonyl)-5-methyl-3-azahexa-1,3,5-triene (11c). The general procedure A was followed using phosphazene **6a** (1.252 g, 4 mmol) and methacrolein **2c** (0.238 mL, 4 mmol) (room temperature/30 h). ^1H NMR (300 MHz, CDCl_3) of crude reaction

mixture (**11c** + Ph₂MePO) δ 1.23 (t, $^3J_{(H,H)} = 7.2$ Hz, 3H), 1.91 (t, $^4J_{(H,H)} = 1.1$ Hz, 3H), 1.96 (d, $^2J_{(P,H)} = 13.0$ Hz, 3H), 4.15 (q, $^3J_{(H,H)} = 7.2$ Hz, 2H), 5.58 (s, 1H), 5.77 (t, $^4J_{(H,H)} = 1.1$ Hz, 1H), 6.03 (d, $^3J_{(H,H)} = 13.3$ Hz, 1H), 7.27-7.09 (m, 10H), 7.76 (d, $^3J_{(H,H)} = 13.3$ Hz, 1H), 7.99 (s, 1H) ppm; ^{13}C NMR (75 MHz, CDCl₃) of crude reaction mixture (**11c** + Ph₂MePO) δ 14.1, 16.4, 16.5 (d, $^1J_{(P,C)} = 74$ Hz), 60.1, 118.1, 128.4-132.4, 133.2, 155.1, 166.8, 170.1 ppm. The general procedure B was followed using phosphazene **6b** (4 mmol), prepared “in situ”, and 0.238 mL (4 mmol) of methacrolein **2c** (room temperature/4 h). ^1H NMR (300 MHz, CDCl₃) of crude reaction mixture (**11c** + Me₃PO) δ 1.23 (t, $^3J_{(H,H)} = 7.2$ Hz, 3H), 1.47 (d, $^2J_{(P,H)} = 12.8$ Hz, 9H), 1.91 (t, $^4J_{(H,H)} = 1.1$ Hz, 3H), 4.15 (q, $^3J_{(H,H)} = 7.2$ Hz, 2H), 5.58 (s, 1H), 5.77 (t, $^4J_{(H,H)} = 1.1$ Hz, 1H), 6.03 (d, $^3J_{(H,H)} = 13.3$ Hz, 1H), 7.76 (d, $^3J_{(H,H)} = 13.3$ Hz, 1H), 7.99 (s, 1H) ppm; ^{13}C NMR (75 MHz, CDCl₃) of crude reaction mixture (**11c** + Me₃PO) δ 14.1, 16.4, 17.8 (d, $^1J_{(P,C)} = 70$ Hz), 60.1, 118.1, 129.4, 133.2, 155.1, 166.8, 170.1 ppm.

1-(Ethoxycarbonyl)-2-phenyl-3-azahepta-1,3,5-triene (11e). The general procedure A was followed using phosphazene **6c** (1.558 g, 4 mmol) and crotonaldehyde **2d** (0.328 mL, 4 mmol) (60 °C/60 h). ^1H NMR (300 MHz, CDCl₃) of crude reaction mixture (**11e** + Ph₂MePO) δ 1.17 (t, $^3J_{(H,H)} = 7.2$ Hz, 3H), 1.86 (d, $^3J_{(H,H)} = 2.1$ Hz, 3H), 1.96 (d, $^2J_{(P,H)} = 13.0$ Hz, 3H), 4.06 (q, $^3J_{(H,H)} = 7.2$ Hz, 2H), 5.66 (s, 1H), 6.31-6.39 (m, 2H), 7.25-7.76 (m, 16H) ppm; ^{13}C NMR (75 MHz, CDCl₃) of crude reaction mixture (**11e** + Ph₂MePO) δ 14.0, 16.5 (d, $^1J_{(P,C)} = 74$ Hz), 18.3, 59.2, 98.3, 125.8-137.2, 144.7, 153.6, 167.6 ppm.

1-(Ethoxycarbonyl)-2,6-diphenyl-3-azahexa-1,3,5-triene (11f). The general procedure A was followed using phosphazene **6c** (1.558 g, 4 mmol) and cinnamaldehyde **2b** (0.504 mL, 4 mmol) (60 °C/16 h). ^1H NMR (300 MHz, CDCl₃) of crude reaction mixture (**11f** + Ph₂MePO) δ 1.18 (t, $^3J_{(H,H)} = 7.2$ Hz, 3H), 1.96 (d, $^2J_{(P,H)}$

= 13.0 Hz, 3H), 4.08 (q, $^3J_{(H,H)} = 7.2$ Hz, 2H), 5.71 (s, 1H), 6.82-7.65 (m, 17H), 7.95 (d, $^3J_{(H,H)} = 8.0$ Hz, 1H) ppm; ^{13}C NMR (75 MHz, CDCl_3) of crude reaction mixture (**11f** + Ph_2MePO) δ 14.2, 16.5 (d, $^1J_{(P,C)} = 74$ Hz), 59.6, 99.0, 126.3-136.6, 145.2, 152.6, 160.0, 166.6 ppm. The general procedure B was followed using phosphazene **6d** (4 mmol), prepared “in situ”, and 0.504 mL (4 mmol) of cinnamaldehyde **2b** (room temperature/24 h). ^1H NMR (300 MHz, CDCl_3) of crude reaction mixture (**11f** + Me_3PO) δ 1.18 (t, $^3J_{(H,H)} = 7.2$ Hz, 3H), 1.47 (d, $^2J_{(P,H)} = 12.8$ Hz, 9H), 4.08 (q, $^3J_{(H,H)} = 7.2$ Hz, 2H), 5.71 (s, 1H), 7.09 (d, $^3J_{(H,H)} = 15.9$ Hz, 1H), 7.29-7.58 (m, 11H), 7.95 (d, $^3J_{(H,H)} = 8.0$ Hz, 1H) ppm; ^{13}C NMR (75 MHz, CDCl_3) of crude reaction mixture (**11f** + Me_3PO) δ 14.2, 17.8 (d, $^1J_{(P,C)} = 70$ Hz), 59.6, 99.0, 126.3-138.1, 145.2, 152.6, 160.0, 166.6 ppm.

1-(Ethoxycarbonyl)-2-phenyl-5-methyl-3-azahexa-1,3,5-triene (11g). The general procedure A was followed using phosphazene **6c** (1.558 g, 4 mmol) and methacrolein **2c** (0.238 mL, 4 mmol) (60 °C/56 h). ^1H NMR (300 MHz, CDCl_3) of crude reaction mixture (**11g** + Ph_2MePO) δ 1.19 (t, $^3J_{(H,H)} = 7.2$ Hz, 3H), 1.96 (d, $^2J_{(P,H)} = 13.0$ Hz, 3H), 2.06 (s, 3H), 4.09 (q, $^3J_{(H,H)} = 7.2$ Hz, 2H), 5.54 (s, 1H), 5.69 (s, 1H), 5.76 (s, 1H), 7.15-7.70 (m, 15H), 7.80 (s, 1H) ppm; ^{13}C NMR (75 MHz, CDCl_3) of crude reaction mixture (**11g** + Ph_2MePO) δ 13.6, 16.2, 16.5 (d, $^1J_{(P,C)} = 74$ Hz), 59.3, 98.4, 125.9-136.3, 164.2, 165.8 ppm.

1-(Ethoxycarbonyl)-2-phenyl-3-azahexa-1,3,5-triene (11h). The general procedure A was followed using phosphazene **6c** (1.558 g, 4 mmol) and acrolein **2a** (0.268 mL, 4 mmol) (room temperature/8 h). ^1H NMR (300 MHz, CDCl_3) of crude reaction mixture (**11h** + Ph_2MePO) δ 1.19 (t, $^3J_{(H,H)} = 7.2$ Hz, 3H), 1.96 (d, $^2J_{(P,H)} = 13.0$ Hz, 3H), 4.07 (q, $^3J_{(H,H)} = 7.2$ Hz, 2H), 5.67 (s, 1H), 5.83 (d, $^3J_{(H,H)} = 17.5$ Hz, 1H), 5.90 (d, $^3J_{(H,H)} = 10.2$ Hz, 1H), 6.30-6.51 (m, 1H), 7.041-7.65 (m, 15H), 7.87 (d, $^3J_{(H,H)} = 9.0$ Hz, 1H)

ppm; ^{13}C NMR (75 MHz, CDCl_3) of crude reaction mixture (**11h** + Ph_2MePO) δ 14.1, 16.5 (d, $^1J_{(\text{P,C})} = 74$ Hz), 59.4, 98.7, 126.2-131.5, 136.0, 144.4, 162.3, 166.1 ppm.

1,2-(Dimethoxycarbonyl)-3-azahepta-1,3,5-triene (11i). The general procedure A was followed using phosphazene **6e** (1.428 g, 4 mmol) and crotonaldehyde **2d** (0.328 mL, 4 mmol) (70 °C/98 h). ^1H NMR (300 MHz, CDCl_3) of crude reaction mixture (**11i** + Ph_2MePO) δ 1.86 (d, $^3J_{(\text{H,H})} = 5.3$ Hz, 3H), 1.96 (d, $^2J_{(\text{P,H})} = 13.0$ Hz, 3H), 3.60 (s, 3H), 3.73 (s, 3H), 6.16 (s, 1H), 6.24-6.32 (m, 1H), 6.37-6.49 (m, 1H), 7.32-7.87 (m, 11H) ppm; ^{13}C NMR (75 MHz, CDCl_3) of crude reaction mixture (**11i** + Ph_2MePO) δ 15.7 (d, $^1J_{(\text{P,C})} = 74$ Hz), 17.8, 50.7, 52.2, 107.5, 122.8-134.1, 145.8, 153.2, 163.2, 164.5 ppm.

Preparation of Pyridines 7 from 3-azatrienes 11.

Ethyl 3-pyridinecarboxylate (7a). The general procedure was followed using 3-azatriene **11a** and acrolein **2a** (0.201 mL, 3 mmol). The mixture was stirred at 60 °C for 34 h, the crude oil was chromatographed on silica gel (10:1 hexane/AcOEt) to give 0.240 g (53%) of **7a** as a yellow oil ($R_f = 0.45$, hexane/AcOEt 2:1) (See the spectroscopy data for the ethyl nicotinate).²

Ethyl 6-phenyl-3-pyridinecarboxylate (7b). The general procedure was following using 3-azatriene **11b** and cinnamaldehyde **2b** (0.378 mL, 3 mmol). The mixture reaction was stirred at 60 °C for 35 h. The crude oil was chromatographed on silica gel (20:1 hexane/AcOEt) to give 0.409 g (60 %) of **7b** as a brown oil ($R_f = 0.49$, hexane/AcOEt 2:1). (See the spectroscopy data for the pyridine **7b**).

Ethyl 5-methyl-3-pyridinecarboxylate (7c). The general procedure was followed using 3-azatriene **11c** and methacrolein **2c** (0.246 mL, 3 mmol). The mixture was stirred

at 60 °C for 36 h, the crude oil was chromatographed on silica gel (10:1 hexane/AcOEt) to give 0.288 g (58%) of **7c** as a yellow oil ($R_f = 0.36$, hexane/AcOEt 2:1) (See the spectroscopy data for the compound **7c**).

Ethyl 6-methyl-3-pyridinecarboxylate (7d). The general procedure was followed using 3-azatriene **11d** and crotonaldehyde **2d** (0.246 mL, 3 mmol). The mixture was stirred at 60 °C for 37 h, the crude oil was chromatographed on silica gel (10:1 hexane/AcOEt) to give 0.296 g (60%) of **7d** as a yellow oil ($R_f = 0.30$, hexane/AcOEt 2:1) (See the spectroscopy data for the compound **7d**).

Ethyl 2,6-diphenyl-3-pyridinecarboxylate (7f). The general procedure was followed using 3-azatriene **11f** and cinnamaldehyde **2b** (0.378 mL, 3 mmol). The mixture was stirred at 90 °C for 60 °C, the crude oil was chromatographed on silica gel (10:1 hexane/AcOEt) to give 0.463 g (51%) of **7f** as a brown oil ($R_f = 0.63$, hexane/AcOEt 2:1). $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 1.00 (t, $^3J_{(\text{H,H})} = 7.2$ Hz, 3H), 4.11 (q, $^3J_{(\text{H,H})} = 7.2$ Hz, 2H), 7.36-7.59 (m, 9H), 7.71 (d, $^3J_{(\text{H,H})} = 8.1$ Hz, 1H), 8.07 (d, $^3J_{(\text{H,H})} = 8.4$ Hz, 1H), 8.11 (d, $^3J_{(\text{H,H})} = 8.1$ Hz, 1H) ppm; $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 13.7, 61.4, 117.8, 125.4, 127.3-129.7, 138.3, 138.9, 140.6, 158.4, 158.6, 168.6 ppm; IR (NaCl) 1720; M/S (EI) m/z 303 (M^+ , 88). Anal. Calcd. for $\text{C}_{20}\text{H}_{17}\text{NO}_2$: C, 79.19; H, 5.65; N, 4.62. Found, C, 79.22; H, 5.67; N, 4.61.

Ethyl 5-methyl-2-phenyl-3-pyridinecarboxylate (7g). The general procedure was followed using 3-azatriene **11g** and methacrolein **2c** (0.246 mL, 3 mmol). The mixture was stirred at 90 °C for 48 h, the crude oil was chromatographed on silica gel (10:1 hexane/AcOEt) to give 0.248 g (50%) of **7g** as a brown oil ($R_f = 0.43$, hexane/AcOEt 2:1). $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 1.33 (t, $^3J_{(\text{H,H})} = 7.2$ Hz, 3H), 2.32 (s, 3H), 4.33 (q, $^3J_{(\text{H,H})} = 7.2$ Hz, 2H), 8.03 (s, 1H), 8.53 (s, 1H) ppm; $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ

14.1, 18.1, 61.2, 126.1, 132.9, 137.2, 147.9, 153.7, 165.4 ppm; IR (NaCl) 1715; M/S (EI) m/z 241 (M^+ , 69). Anal. Calcd. for $C_{15}H_{15}NO_2$: C, 74.67; H, 6.27; N, 8.51. Found: C, 74.70; H, 6.28; N, 8.49.

Ethyl 6-methyl-3-pyridinecarboxylate (7b). The general procedure was following using 3-azatriene **11c** and crotonaldehyde **2d** (0.246 mL, 3 mmol). the mixture was stirred at 60 °C for 46 h. Evaporation of solvent under reduced pressure afforded an oil which was chromatographed on silica gel (10:1 hexane/AcOEt) to give 0.188 g (38%) of **7b** as a yellow oil ($R_f = 0.30$, Hexane/AcOEt 2:1) (See the spectroscopy data for pyridine **7d**).

Ethyl 6-phenyl-3-pyridinecarboxylate (7c). The general procedure was following using 3-azatriene **11d** and cinnamaldehyde **2b** (0.378 mL, 3 mmol). the mixture was stirred at 60 °C for 48 h. Evaporation of solvent under reduced pressure afforded an oil which was chromatographed on silica gel (20:1 hexane/AcOEt) to give 0.238 g (35%) of **7c** as a yellow oil ($R_f = 0.52$, Hexane/AcOEt 2:1) (See the spectroscopy data for pyridine **7b**).

Table 1. Total Energies (hartree) and zero-point vibrational energies (hartree/particle), of all Stationary Points Discussed in This Work

B3LYP/6-31G*	Energy	ZPVE
2a	-191.91197	0.06165
2e	-114.50047	0.02683
6f	-475.84376	0,07521
6g	-589.17872	0.08563
6h	-593.83292	0.16221

6i	-707.17237	0.17265
6j	-821.72412	0.20592
6k	-861.04159	0.23395
6l	-1396.91948	0.36720
6m	-1436.23401	0.39511
6n	-1013.45778	0.25987
6o	-1052.77470	0.28748
6p	-1205.18833	0.31378
6q	-1244.50292	0.34150
TS1_{22a}	-590.33761	0.10558
TS1_{22b}	-703.67110	0.11608
TS1_{22c}	-708.32807	0.19324
TS1_{22d}	-821.66327	0.20399
TS1_{22e}	-899.06129	0.23660
TS1_{22f}	-936.21814	0.23756
TS1_{22g}	-1013.61703	0.27057
TS1_{22h}	-975.52818	0.26560
TS1_{22i}	-1052.91966	0.29911
TS1_{22j}	-1511.40782	0.39814
TS1_{22k}	-1550.71682	0.42632
TS1_{22l}	-1127.94967	0.29190
TS1_{22m}	-1167.25848	0.31991
TS1_{22n}	-1244.65588	0.35353
TS1_{22o}	-1319.67890	0.34529
TS1_{22p}	-1358.98775	0.37303

TS1_{42a}	-590.34487	0.10711
TS1_{42b}	-703.67344	0.11758
TS1_{42c}	-708.33393	0.19405
TS1_{42d}	-821.65831	0.20430
TS1_{42e}	-899.05595	0.23728
TS1_{42f}	-936.21540	0.23817
TS1_{42g}	-1013.60651	0.27104
TS1_{42h}	-975.53482	0.26591
TS1_{42i}	-1052.93170	0.29861
TS1_{42j}	-1511.40522	0.39828
TS1_{42k}	-1550.72495	0.42599
TS1_{42l}	-1127.94599	0.29183
TS1_{42m}	-1167.26550	0.31968
TS1_{42n}	-1244.66215	0.35260
TS1_{42o}	-1319.67496	0.34503
TS1_{42p}	-1358.99763	0.37286
INT_{22a}	-590.38325	0.11050
INT_{22b}	-703.71394	0.12055
INT_{22c}	-708.35311	0.19656
INT_{22d}	-821.69209	0.20698
INT_{22e}	-899.08957	0.23963
INT_{22f}	-936.24607	0.24049
INT_{22g}	-1013.63884	0.27327
INT_{22h}	-975.55888	0.26869
INT_{22i}	-1052.95720	0.30168

INT_{22j}	-1511.43453	0.40094
INT_{22k}	-1550.74759	0.42898
INT_{22l}	-1127.97306	0.29420
INT_{22m}	-1167.28543	0.32236
INT_{22n}	-1244.67906	0.35526
INT_{22o}	-1319.70375	0.34778
INT_{22p}	-1359,01793	0.37580
INT_{42a}	-590.38626	0.11159
INT_{42b}	-703.69731	0.12059
INT_{42c}	-708.35204	0.19768
INT_{42d}	-821.66524	0.20662
INT_{42e}	-899.05316	0.23946
INT_{42f}	-936.22146	0.24060
INT_{42g}	-1013.61863	0.27380
INT_{42h}	-975.54666	0.26870
INT_{42i}	-1052.93649	0.30141
INT_{42j}	-1511.41484	0.40100
INT_{42k}	-1550.73732	0.42891
INT_{42l}	-1127.95228	0.29399
INT_{42m}	-1167.27540	0.32229
INT_{42n}	-1244.66548	0.35461
INT_{42o}	-1319.68014	0.34772
INT_{42p}	-1359.00910	0.37548
TS_{22a}	-590.35458	0.10814
11k	-172.02802	0.07351

11l	-285.35242	0.08332
11m	-362.76352	0.11700
11n	-399.90720	0.11760
11o	-439.22736	0.14569
11p	-516.63604	0.17916
15a	-418.35772	0.03122
15b	-536.35299	0.11809
15c	-1111.55043	0.27917
15d	-728.08653	0.17182
15e	-919.81857	0.22556

2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.677138	0.351064	0.000000
2	8	0	1.796503	-0.122451	0.000000
3	6	0	-0.562501	-0.448075	0.000000
4	1	0	0.517882	1.453493	0.000000
5	6	0	-1.764321	0.140080	0.000000
6	1	0	-0.442878	-1.529081	0.000000
7	1	0	-2.689890	-0.427848	0.000000
8	1	0	-1.859030	1.224627	0.000000

2e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.528887	0.000000	-0.000001
2	8	0	-0.677561	0.000000	0.000000
3	1	0	1.123587	-0.937759	0.000003
4	1	0	1.123579	0.937765	0.000003

6f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.089784	-0.880835	-0.000061
2	6	0	1.259890	-0.543127	0.000022
3	6	0	1.847732	0.666734	-0.000012
4	15	0	-1.254787	0.184396	0.000012
5	1	0	1.895933	-1.429630	0.000120
6	1	0	1.284234	1.599352	-0.000118
7	1	0	2.928900	0.754446	0.000065

8	1	0	-1.407658	1.106952	1.081071
9	1	0	-2.489128	-0.479903	0.000009
10	1	0	-1.407716	1.107048	-1.080956

6g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.936080	-0.079404	-0.000002
2	6	0	0.035947	0.942842	0.000000
3	7	0	-1.333108	0.914559	-0.000003
4	15	0	-2.174122	-0.436973	0.000001
5	1	0	0.428780	1.962275	0.000005
6	1	0	0.631794	-1.126554	-0.000006
7	6	0	2.362980	0.180686	0.000001
8	1	0	-2.060464	-1.348108	-1.087620
9	1	0	-3.537856	-0.119459	0.000000
10	1	0	-2.060464	-1.348102	1.087627
11	8	0	3.237484	-0.674459	0.000000
12	1	0	2.631875	1.263555	0.000006

6h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.643233	0.422496	-0.000082
2	6	0	-2.008184	-0.767719	-0.000218
3	7	0	-0.660101	-1.082923	-0.000527
4	15	0	0.554511	-0.064417	-0.000026
5	6	0	0.714256	1.066615	-1.450480
6	6	0	2.088964	-1.049674	-0.000333
7	6	0	0.713833	1.065352	1.451443
8	1	0	-3.727550	0.463263	0.000179
9	1	0	-2.121895	1.377858	-0.000292
10	1	0	-2.633079	-1.664432	-0.000083
11	1	0	1.608544	1.694888	-1.377523
12	1	0	0.768309	0.466998	-2.364140
13	1	0	-0.170233	1.706338	-1.515200
14	1	0	2.974125	-0.405687	0.000620
15	1	0	2.102619	-1.690078	0.885773
16	1	0	2.103384	-1.688467	-0.887591
17	1	0	1.607002	1.695190	1.378319
18	1	0	-0.171691	1.703497	1.517569
19	1	0	0.769696	0.464918	2.364458

6i

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.771781	-0.459624	0.000000
2	6	0	-3.196178	-0.701947	0.000000
3	8	0	-3.734811	-1.803302	0.000000
4	6	0	-1.275898	0.816232	0.000000
5	7	0	0.000000	1.286152	0.000000
6	15	0	1.333881	0.396319	0.000000
7	1	0	-2.017702	1.620926	0.000000
8	1	0	-1.131153	-1.340047	0.000000
9	6	0	1.590449	-0.692326	1.459036
10	6	0	2.732022	1.562105	0.000000
11	6	0	1.590449	-0.692326	-1.459036
12	1	0	-3.817845	0.226380	0.000000

13	1	0	3.689661	1.032423	0.000000
14	1	0	2.665946	2.198325	-0.886772
15	1	0	2.665946	2.198325	0.886772
16	1	0	2.553624	-1.210220	-1.403204
17	1	0	0.786691	-1.431346	-1.514146
18	1	0	1.560205	-0.083662	-2.367622
19	1	0	2.553624	-1.210220	1.403204
20	1	0	1.560205	-0.083662	2.367622
21	1	0	0.786691	-1.431346	1.514146

6j

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.744363	1.028549	-1.447928
2	15	0	2.381506	-0.048873	-0.000016
3	6	0	2.745064	1.025001	1.450357
4	7	0	0.965225	-0.784221	-0.000456
5	6	0	-0.232850	-0.123066	-0.000320
6	6	0	-1.444888	-0.736591	-0.000204
7	6	0	-2.656951	0.068546	-0.000096
8	8	0	-2.731982	1.290384	-0.000114
9	6	0	3.660863	-1.342254	-0.001820
10	8	0	-3.774504	-0.722903	0.000063
11	6	0	-5.014074	-0.013497	0.000225
12	1	0	3.753050	1.452199	-1.395709
13	1	0	2.643655	0.442199	-2.365995
14	1	0	2.017722	1.846687	-1.482962
15	1	0	3.753872	1.448465	1.398930
16	1	0	2.018668	1.843263	1.487520
17	1	0	2.644382	0.436475	2.367036
18	1	0	-0.264912	0.972871	-0.000350
19	1	0	-1.532042	-1.817380	-0.000164
20	1	0	4.664767	-0.906721	-0.001272
21	1	0	3.533653	-1.970285	0.884054
22	1	0	3.533598	-1.967959	-0.889332
23	1	0	-5.793192	-0.778368	0.000271
24	1	0	-5.104737	0.620555	0.887841
25	1	0	-5.104921	0.620645	-0.887305

6k

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.096845	-1.335983	1.460617
2	15	0	2.207405	-0.221150	0.000003
3	6	0	2.096937	-1.336009	-1.460598
4	7	0	1.261110	1.066482	-0.000047
5	6	0	-0.109194	1.108929	-0.000039
6	6	0	-0.941164	0.013006	-0.000038
7	6	0	-2.388372	0.069471	0.000003
8	8	0	-3.115825	1.053701	0.000074
9	6	0	3.920920	0.397378	0.000054
10	6	0	-0.654563	2.522032	-0.000035
11	8	0	-2.911567	-1.205388	-0.000042
12	6	0	-4.337645	-1.266450	0.000006
13	1	0	2.832403	-2.144996	1.399275
14	1	0	2.280718	-0.750236	2.366290
15	1	0	1.093910	-1.764895	1.528549
16	1	0	2.832390	-2.145108	-1.399135
17	1	0	1.093959	-1.764805	-1.528652
18	1	0	2.280999	-0.750308	-2.366261
19	1	0	-0.525798	-0.990058	-0.000064
20	1	0	4.639942	-0.427845	0.000011

21	1	0	4.076561	1.017978	-0.886556
22	1	0	4.076553	1.017876	0.886738
23	1	0	0.177822	3.228925	-0.000274
24	1	0	-1.291651	2.696030	0.872246
25	1	0	-1.292078	2.695889	-0.872025
26	1	0	-4.589213	-2.329228	-0.000013
27	1	0	-4.754372	-0.779066	0.887215
28	1	0	-4.754434	-0.779022	-0.887149

6l

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.395238	0.238592	-0.332269
2	6	0	2.233128	0.005231	-1.082545
3	6	0	2.331446	-0.220437	-2.461771
4	6	0	3.582565	-0.217238	-3.080655
5	6	0	4.737046	0.011085	-2.330300
6	6	0	4.642285	0.239979	-0.955301
7	15	0	0.586927	-0.010430	-0.294365
8	6	0	0.579421	-1.426886	0.871074
9	6	0	1.345289	-2.566699	0.577068
10	6	0	1.256590	-3.702958	1.380205
11	6	0	0.398031	-3.717515	2.481025
12	6	0	-0.373068	-2.592336	2.777127
13	6	0	-0.286252	-1.453176	1.977102
14	6	0	0.478124	1.508914	0.730452
15	6	0	-0.153249	2.623893	0.158902
16	6	0	-0.227484	3.825481	0.862742
17	6	0	0.328766	3.925299	2.139383
18	6	0	0.956804	2.819412	2.715674
19	6	0	1.030451	1.614021	2.016713
20	7	0	-0.454443	-0.096247	-1.509165
21	6	0	-1.816631	-0.136335	-1.461862
22	6	0	-2.669775	0.028685	-0.410798
23	6	0	-4.120242	-0.035412	-0.511897
24	8	0	-4.889651	0.115292	0.425417
25	1	0	-2.267001	-0.317357	-2.438199
26	1	0	-2.312680	0.234577	0.592309
27	8	0	-4.571215	-0.285810	-1.782042
28	1	0	-0.888888	-0.584854	2.222291
29	1	0	-1.047043	-2.599799	3.629074
30	1	0	0.328191	-4.604224	3.105221
31	1	0	1.858196	-4.576640	1.145075
32	1	0	2.012198	-2.566088	-0.279601
33	1	0	1.503923	0.754221	2.482096
34	1	0	1.384090	2.891910	3.712122
35	1	0	0.267650	4.861541	2.687518
36	1	0	-0.725377	4.681472	0.416075
37	1	0	-0.593779	2.539560	-0.829829
38	1	0	1.420683	-0.386858	-3.027115
39	1	0	3.653505	-0.391307	-4.150876
40	1	0	5.709737	0.014467	-2.815001
41	1	0	5.538442	0.423270	-0.368955
42	1	0	3.331924	0.426513	0.735758
43	6	0	-5.991979	-0.353012	-1.911835
44	1	0	-6.182786	-0.553834	-2.967959
45	1	0	-6.406277	-1.154471	-1.292406
46	1	0	-6.459606	0.590701	-1.614367

6m

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.501048	0.064535	-0.188463

2	6	0	2.356334	-0.164295	-0.966530
3	6	0	2.494309	-0.490175	-2.321799
4	6	0	3.765655	-0.588815	-2.889607
5	6	0	4.902119	-0.364067	-2.111390
6	6	0	4.768571	-0.037194	-0.759579
7	15	0	0.682569	-0.032262	-0.246230
8	6	0	0.587311	-1.290725	1.085894
9	6	0	1.312962	-2.486351	0.956239
10	6	0	1.161819	-3.509499	1.891333
11	6	0	0.278799	-3.355277	2.961703
12	6	0	-0.453510	-2.174651	3.094694
13	6	0	-0.303689	-1.147581	2.162701
14	6	0	0.616276	1.605386	0.585550
15	6	0	0.046023	2.667145	-0.132332
16	6	0	0.010572	3.948286	0.417320
17	6	0	0.545341	4.180965	1.685746
18	6	0	1.112587	3.128988	2.407548
19	6	0	1.147262	1.845052	1.862448
20	7	0	-0.317484	-0.232942	-1.475078
21	6	0	-1.690894	-0.287725	-1.501009
22	6	0	-2.499183	0.084159	-0.455885
23	6	0	-3.945231	0.078146	-0.281016
24	8	0	-4.487853	0.454607	0.749554
25	6	0	-2.190491	-0.791086	-2.836939
26	1	0	-2.025217	0.472734	0.438781
27	8	0	-4.685362	-0.382905	-1.337038
28	1	0	-0.879144	-0.235722	2.282470
29	1	0	-1.146843	-2.050898	3.921775
30	1	0	0.160297	-4.153938	3.689003
31	1	0	1.733865	-4.426895	1.782759
32	1	0	1.999142	-2.616911	0.125023
33	1	0	1.572273	1.029905	2.441029
34	1	0	1.521923	3.305296	3.398592
35	1	0	0.514271	5.178919	2.114570
36	1	0	-0.440700	4.762679	-0.142438
37	1	0	-0.379385	2.479351	-1.113604
38	1	0	1.597278	-0.655606	-2.908996
39	1	0	3.866622	-0.840429	-3.941901
40	1	0	5.890819	-0.440552	-2.556079
41	1	0	5.650734	0.141892	-0.151067
42	1	0	3.408840	0.326650	0.861646
43	6	0	-6.099103	-0.382505	-1.122838
44	1	0	-6.535582	-0.769762	-2.045572
45	1	0	-6.367533	-1.022176	-0.276889
46	1	0	-6.465956	0.628549	-0.922856
47	1	0	-3.274538	-0.777840	-2.912299
48	1	0	-1.754417	-0.176725	-3.633568
49	1	0	-1.826500	-1.813888	-2.994227

6n

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.487083	-1.586621	-1.456890
2	15	0	-0.725485	-0.486719	0.000117
3	6	0	-0.487211	-1.586283	1.457382
4	7	0	0.108242	0.878866	0.000135
5	6	0	1.463726	1.010267	0.000231
6	6	0	2.451995	0.068924	-0.000152
7	6	0	3.849159	0.475811	0.000059
8	8	0	4.289895	1.615035	0.000685
9	6	0	-2.482773	-0.020136	-0.000037
10	8	0	4.674327	-0.621013	-0.000560
11	6	0	-3.491275	-0.995928	0.000160
12	6	0	-4.833247	-0.617780	0.000067
13	6	0	-5.175774	0.736492	-0.000238
14	6	0	-4.175636	1.710220	-0.000438

15	6	0	-2.831029	1.336810	-0.000331
16	6	0	6.071041	-0.319541	-0.000386
17	1	0	-1.153568	-2.453880	-1.416233
18	1	0	0.550184	-1.930774	-1.493803
19	1	0	-0.697753	-1.014503	-2.364678
20	1	0	-1.152901	-2.454141	1.416362
21	1	0	-0.698965	-1.014266	2.364980
22	1	0	0.550338	-1.929513	1.494987
23	1	0	1.799231	2.048690	0.000680
24	1	0	2.251696	-0.998600	-0.000703
25	1	0	-3.239384	-2.053906	0.000395
26	1	0	-5.609449	-1.377959	0.000229
27	1	0	-6.221866	1.030715	-0.000318
28	1	0	-4.441289	2.763726	-0.000675
29	1	0	-2.037303	2.076568	-0.000458
30	1	0	6.348907	0.256651	0.887664
31	1	0	6.348749	0.258410	-0.887333
32	1	0	6.582817	-1.284079	-0.001366

60

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.567859	-1.662781	1.459190
2	15	0	0.811306	-0.566801	-0.000950
3	6	0	0.570498	-1.667594	-1.457910
4	7	0	0.001477	0.810586	-0.004048
5	6	0	-1.354571	1.003458	-0.003079
6	6	0	-2.301020	0.005041	-0.001829
7	6	0	-3.733576	0.219863	0.000860
8	8	0	-4.348187	1.278273	0.005080
9	6	0	2.577099	-0.125132	-0.000129
10	6	0	-1.744830	2.467198	-0.002228
11	8	0	-4.393539	-0.989332	-0.001682
12	6	0	3.570981	-1.115974	0.001484
13	6	0	4.918793	-0.758808	0.002345
14	6	0	5.282690	0.589782	0.001597
15	6	0	4.297566	1.578622	-0.000009
16	6	0	2.947424	1.225748	-0.000868
17	6	0	-5.817778	-0.893263	0.001153
18	1	0	1.234552	-2.529914	1.420174
19	1	0	-0.469011	-2.006879	1.499067
20	1	0	0.780864	-1.088095	2.364885
21	1	0	1.237711	-2.534176	-1.415404
22	1	0	0.784202	-1.095585	-2.365133
23	1	0	-0.466083	-2.012565	-1.498003
24	1	0	-1.997606	-1.036967	-0.003220
25	1	0	-2.382362	2.703985	-0.858771
26	1	0	-0.842448	3.081973	-0.027201
27	1	0	-2.336275	2.713449	0.884853
28	1	0	3.303541	-2.170115	0.002071
29	1	0	5.682885	-1.531187	0.003585
30	1	0	6.333235	0.867714	0.002267
31	1	0	4.579348	2.627975	-0.000595
32	1	0	2.165431	1.977707	-0.002121
33	1	0	-6.179814	-0.361023	-0.884254
34	1	0	-6.176558	-0.364921	0.890208
35	1	0	-6.184531	-1.921942	-0.000476

6p

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.320398	-0.956430	0.079536

2	15	0	-0.643899	-0.359773	0.468848
3	6	0	-0.579792	1.417525	0.022392
4	6	0	-0.499775	-0.432577	2.301380
5	7	0	0.361632	-1.312569	-0.335758
6	6	0	1.725756	-1.255888	-0.306035
7	6	0	2.556590	-0.356721	-0.296225
8	6	0	4.009848	-0.421651	0.250073
9	8	0	4.488052	-1.490913	-0.462558
10	6	0	5.912155	-1.581193	-0.525472
11	8	0	4.759389	0.381111	0.785470
12	1	0	2.195384	-2.065420	-0.865073
13	1	0	2.177815	0.497611	0.849756
14	1	0	-1.310051	0.106626	2.800252
15	1	0	-0.550062	-1.485897	2.591487
16	1	0	0.463600	-0.025127	-2.618397
17	1	0	6.125429	-2.472444	-1.119031
18	1	0	6.342081	-0.695316	-1.003054
19	1	0	6.344954	-1.678920	0.474935
20	6	0	-0.163645	1.740514	-1.278527
21	6	0	-0.103163	3.071930	-1.686478
22	6	0	-0.454699	4.092901	-0.800891
23	6	0	-0.862339	3.780780	0.496791
24	6	0	-0.922310	2.448911	0.909674
25	1	0	0.126118	0.945681	-1.959508
26	1	0	0.226292	3.312644	-2.693275
27	1	0	-0.403309	5.130578	-1.118936
28	1	0	-1.126717	4.573080	1.191713
29	1	0	-1.228043	2.225642	1.927774
30	6	0	-2.473844	-2.152182	-0.633925
31	6	0	-3.752857	-2.633833	-0.916463
32	6	0	-4.879585	-1.928547	-0.490325
33	6	0	-4.729873	-0.733278	0.217097
34	6	0	-3.454532	-0.246232	0.499862
35	1	0	-1.584964	-2.680765	-0.961960
36	1	0	-3.868128	-3.560571	-1.471896
37	1	0	-5.874150	-2.306011	-0.712475
38	1	0	-5.605049	-0.177958	0.542928
39	1	0	-3.348878	0.695382	1.032775

6q

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.709675	1.483981	-0.022619
2	15	0	0.727534	-0.283298	0.470218
3	6	0	2.416819	-0.897942	0.164035
4	6	0	0.518615	-0.309296	2.298111
5	7	0	-0.246517	-1.245122	-0.353141
6	6	0	-1.622609	-1.244235	-0.368687
7	6	0	-2.403829	-0.273600	0.209700
8	6	0	-3.847961	-0.131004	0.327990
9	8	0	-4.598324	-1.168763	-0.159640
10	6	0	-6.011947	-0.997822	-0.027819
11	8	0	-4.380717	0.840917	0.846835
12	6	0	-2.162516	-2.449813	-1.106565
13	1	0	-1.911483	0.580265	0.666215
14	1	0	1.318194	0.233491	2.810032
15	1	0	-0.450337	0.113419	2.574769
16	1	0	0.550315	-1.356181	2.613248
17	1	0	-6.457566	-1.896275	-0.459389
18	1	0	-6.298028	-0.898097	1.023364
19	1	0	-6.352664	-0.107736	-0.565161
20	6	0	2.594700	-2.108272	-0.517974
21	6	0	3.881651	-2.603335	-0.733483
22	6	0	4.993032	-1.896718	-0.270831
23	6	0	4.819552	-0.686653	0.405273
24	6	0	3.536069	-0.186267	0.620225

25	1	0	1.717431	-2.637727	-0.874539
26	1	0	4.015251	-3.541689	-1.264902
27	1	0	5.993994	-2.284621	-0.440082
28	1	0	5.682927	-0.130102	0.759379
29	1	0	3.413151	0.766853	1.128506
30	6	0	0.402797	1.774161	-1.361193
31	6	0	0.382643	3.094111	-1.807730
32	6	0	0.665301	4.137307	-0.923161
33	6	0	0.963549	3.858294	0.411089
34	6	0	0.983881	2.537423	0.862063
35	1	0	0.165317	0.962109	-2.042323
36	1	0	0.138147	3.309154	-2.844176
37	1	0	0.644898	5.166405	-1.271222
38	1	0	1.173006	4.667921	1.104778
39	1	0	1.203527	2.340538	1.907324
40	1	0	-3.211162	-2.344066	-1.373525
41	1	0	-1.555636	-2.613925	-2.003042
42	1	0	-2.050880	-3.343555	-0.478661

TS1_{22a}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.803921	1.576779	0.027774
2	8	0	1.926136	1.022531	-0.029364
3	1	0	0.348234	2.048101	-0.861871
4	1	0	0.399556	1.962534	0.981391
5	7	0	-0.358091	-0.060147	0.004664
6	15	0	0.842798	-1.145281	-0.001037
7	6	0	-1.713907	-0.399376	-0.008838
8	6	0	-2.707475	0.499286	-0.016937
9	1	0	0.230527	-2.419106	0.001487
10	1	0	1.704450	-1.251345	1.104386
11	1	0	1.699966	-1.253845	-1.109438
12	1	0	-1.964533	-1.463649	0.038556
13	1	0	-3.740102	0.169485	-0.006767
14	1	0	-2.517743	1.567692	-0.047977

TS1_{22b}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.667118	1.625824	0.029652
2	8	0	2.794557	1.079861	-0.035610
3	7	0	0.571786	-0.066210	0.001224
4	6	0	-0.729973	-0.505796	0.005080
5	6	0	-1.811669	0.312580	-0.005957
6	15	0	1.861334	-1.077378	0.000487
7	1	0	1.200798	2.089863	-0.856463
8	1	0	1.258321	1.990048	0.988207
9	1	0	1.304720	-2.376125	0.000862
10	1	0	2.703177	-1.141048	1.120306
11	1	0	2.707966	-1.143338	-1.114911
12	1	0	-0.912374	-1.585817	0.018857
13	6	0	-3.148426	-0.254961	0.002024
14	1	0	-1.712807	1.394087	-0.022448
15	8	0	-4.189882	0.383007	-0.008704
16	1	0	-3.172021	-1.372344	0.019435

TS1_{22c}

Center	Atomic	Atomic	Coordinates (Angstroms)		
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Number	Number	Type	X	Y	Z
1	6	0	1.043426	1.711460	-0.000072
2	8	0	-0.110997	2.266582	0.000121
3	1	0	1.684160	1.785984	0.907652
4	1	0	1.684030	1.786366	-0.907852
5	7	0	0.806307	-0.011715	-0.000385
6	6	0	1.831073	-0.957132	-0.000061
7	6	0	3.140837	-0.665756	0.000033
8	15	0	-0.808360	-0.314343	-0.000015
9	6	0	-1.070644	-2.127737	-0.000233
10	6	0	-1.680010	0.290094	-1.484870
11	6	0	-1.679474	0.289628	1.485363
12	1	0	1.528433	-2.004759	0.000094
13	1	0	3.868477	-1.469408	0.000261
14	1	0	3.517403	0.350783	-0.000139
15	1	0	-2.146713	-2.329101	-0.000248
16	1	0	-0.630857	-2.585987	-0.890435
17	1	0	-0.630851	-2.586226	0.889842
18	1	0	-2.752535	0.076253	-1.417682
19	1	0	-1.492439	1.364932	-1.529769
20	1	0	-1.264036	-0.203601	-2.368731
21	1	0	-1.492193	1.364511	1.530354
22	1	0	-2.751969	0.075473	1.418687
23	1	0	-1.262913	-0.204074	2.368945

TS1₂₂d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.515440	2.080707	-0.000003
2	8	0	1.795316	2.024640	-0.000201
3	1	0	-0.017170	2.442120	-0.907805
4	1	0	-0.016858	2.441859	0.908088
5	7	0	-0.046053	0.438732	-0.000117
6	6	0	-1.344327	0.014844	-0.000066
7	6	0	-2.439036	0.822943	0.000012
8	15	0	1.299403	-0.545687	0.000012
9	6	0	0.717682	-2.281862	0.000270
10	6	0	2.327212	-0.400071	1.498737
11	6	0	2.327305	-0.400674	-1.498717
12	6	0	-3.762694	0.215327	0.000000
13	8	0	-3.995668	-0.989497	-0.000042
14	1	0	-1.546006	-1.056388	-0.000132
15	1	0	-2.361547	1.905325	0.000066
16	1	0	1.590480	-2.942677	0.000576
17	1	0	0.118788	-2.496558	0.889618
18	1	0	0.119116	-2.496937	-0.889206
19	1	0	3.164190	-1.105352	1.449227
20	1	0	2.676670	0.632119	1.546346
21	1	0	1.710916	-0.631601	2.373107
22	1	0	2.677330	0.631309	-1.546446
23	1	0	3.163851	-1.106468	-1.449240
24	1	0	1.710821	-0.631829	-2.373056
25	1	0	-4.605934	0.940832	0.000032

TS1₂₂e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.447263	1.659592	0.561060
2	8	0	1.716246	1.536868	0.715284
3	6	0	-0.037234	2.609180	-0.499332
4	6	0	-0.990447	3.518666	-0.291985

5	1	0	-0.208357	1.687289	1.457737
6	1	0	0.510439	2.572501	-1.440174
7	1	0	-1.271877	4.247175	-1.047570
8	1	0	-1.518428	3.577801	0.658564
9	7	0	-0.019880	0.034285	-0.019815
10	6	0	-1.256085	-0.553484	-0.020678
11	6	0	-2.449755	0.084284	0.116865
12	15	0	1.420163	-0.822726	-0.066372
13	6	0	1.001151	-2.515290	-0.647652
14	6	0	2.267712	-1.141381	1.523505
15	6	0	2.595076	-0.232301	-1.331194
16	6	0	-3.671756	-0.707554	0.104726
17	8	0	-3.734755	-1.928382	-0.007420
18	1	0	-1.319969	-1.635769	-0.134935
19	1	0	-2.523192	1.160945	0.214613
20	1	0	1.931276	-3.075100	-0.789237
21	1	0	0.388271	-3.050056	0.082922
22	1	0	0.464132	-2.481764	-1.599552
23	1	0	3.062394	-1.882154	1.380053
24	1	0	2.659982	-0.198324	1.900201
25	1	0	1.534232	-1.542590	2.230493
26	1	0	2.906804	0.775205	-1.060113
27	1	0	3.452658	-0.912473	-1.381632
28	1	0	2.088758	-0.224644	-2.301466
29	1	0	-4.607875	-0.115308	0.209590

TS1₂₂f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.721481	-2.269496	-0.002756
2	15	0	-2.154093	-0.490317	-0.000228
3	6	0	-3.167341	-0.257508	1.497753
4	7	0	-0.736968	0.378335	-0.002744
5	6	0	0.526340	-0.154466	-0.001247
6	6	0	1.676506	0.561790	-0.001754
7	6	0	2.943140	-0.167127	-0.000038
8	8	0	3.082782	-1.381707	0.001973
9	6	0	-1.152309	2.060866	0.000030
10	8	0	-2.432397	2.122514	0.002547
11	6	0	-3.172750	-0.254276	-1.493912
12	1	0	-0.587990	2.373204	0.907090
13	1	0	-0.591488	2.375590	-0.908345
14	1	0	0.634304	-1.238437	0.000404
15	1	0	1.701280	1.644472	-0.003535
16	1	0	-2.646977	-2.854289	-0.003139
17	1	0	-1.143211	-2.532205	-0.892828
18	1	0	-1.142477	-2.534706	0.886098
19	1	0	-4.074193	-0.874500	-1.438104
20	1	0	-3.421026	0.807154	-1.540461
21	1	0	-2.586853	-0.544674	-2.371581
22	1	0	-3.418710	0.803115	1.545715
23	1	0	-4.066926	-0.880772	1.445984
24	1	0	-2.576631	-0.545888	2.372864
25	8	0	4.001650	0.690106	-0.000984
26	6	0	5.288698	0.064102	0.000516
27	1	0	6.013041	0.880165	-0.000471
28	1	0	5.418109	-0.559827	0.889877
29	1	0	5.418825	-0.562605	-0.886787

TS1₂₂g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	1.315489	-2.560943	-0.897070
2	15	0	1.895969	-1.038065	-0.051410
3	6	0	3.248951	-0.445935	-1.119839
4	7	0	0.587030	-0.003150	0.018903
5	6	0	-0.720620	-0.401194	-0.090436
6	6	0	-1.810333	0.376218	0.124786
7	6	0	-3.131356	-0.226748	-0.038948
8	8	0	-3.369565	-1.381536	-0.361982
9	6	0	2.546847	-1.656661	1.540960
10	8	0	-4.116621	0.677576	0.220973
11	6	0	-5.450517	0.175713	0.090820
12	1	0	2.169914	-3.230041	-1.041246
13	1	0	0.564651	-3.088538	-0.302939
14	1	0	0.887802	-2.322133	-1.874781
15	1	0	3.721395	0.402965	-0.628356
16	1	0	3.960886	-1.260456	-1.293423
17	1	0	2.823853	-0.125093	-2.075263
18	1	0	-0.925520	-1.432329	-0.375876
19	1	0	-1.752895	1.416864	0.417572
20	1	0	3.341594	-2.389318	1.360793
21	1	0	2.913673	-0.799121	2.103758
22	1	0	1.732102	-2.142649	2.087486
23	1	0	-6.105553	1.014870	0.330463
24	1	0	-5.637575	-0.175439	-0.928322
25	1	0	-5.624535	-0.653696	-0.782772
26	6	0	1.202167	1.473920	0.748042
27	8	0	2.404596	1.176965	1.091330
28	6	0	0.976657	2.510310	-0.330996
29	6	0	1.966844	3.284505	-0.773589
30	1	0	0.433248	1.568092	1.547319
31	1	0	-0.040784	2.630687	-0.702061
32	1	0	2.968772	3.163948	-0.370826
33	1	0	1.808179	4.055264	-1.523190

TS1₂₂h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.996112	-1.731257	1.452995
2	15	0	-1.839550	-0.695255	0.190617
3	6	0	-3.510332	-0.524832	0.908182
4	7	0	-1.012460	0.757409	0.165338
5	6	0	0.362883	0.953710	0.252986
6	6	0	0.715038	2.334196	0.748301
7	6	0	-1.999903	1.782370	-0.821617
8	1	0	-2.297716	2.557481	-0.083554
9	8	0	-2.900146	1.002773	-1.304705
10	6	0	1.286288	0.021505	-0.123871
11	6	0	2.739923	0.132758	-0.004014
12	8	0	3.319211	-1.013347	-0.477570
13	6	0	4.749612	-1.032106	-0.432523
14	6	0	-1.902491	-1.747110	-1.307156
15	8	0	3.410533	1.053660	0.435538
16	1	0	-1.222217	2.195019	-1.501773
17	1	0	0.954499	-0.907612	-0.573444
18	1	0	-1.021999	-1.214328	2.416822
19	1	0	-1.533079	-2.680718	1.548925
20	1	0	0.044214	-1.934922	1.198676
21	1	0	-2.468914	-2.660923	-1.094284
22	1	0	-2.382757	-1.165684	-2.094049
23	1	0	-0.887603	-2.022483	-1.609415
24	1	0	-4.206090	-0.216292	0.131464
25	1	0	-3.806735	-1.469657	1.377523
26	1	0	-3.469002	0.255629	1.673604
27	1	0	0.247140	2.508913	1.724006
28	1	0	1.793269	2.462550	0.822790
29	1	0	0.308117	3.086780	0.060602

30	1	0	5.044071	-1.999267	-0.843336
31	1	0	5.169465	-0.219290	-1.032333
32	1	0	5.109592	-0.928329	0.595358

TS1₂₂i

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.174519	0.985964	0.733544
2	8	0	2.680730	-0.039344	1.344202
3	6	0	3.025151	1.614884	-0.351276
4	6	0	3.145577	2.920560	-0.596619
5	1	0	1.672157	1.767529	1.337030
6	1	0	3.644764	0.911748	-0.906087
7	1	0	3.828492	3.295286	-1.355904
8	1	0	2.576497	3.668555	-0.049012
9	7	0	0.811480	0.281926	-0.070715
10	6	0	-0.480268	0.784829	0.022994
11	6	0	-1.604780	0.015857	0.183238
12	15	0	1.214887	-1.363561	-0.102182
13	6	0	0.226308	-2.057952	-1.496138
14	6	0	0.826967	-2.386875	1.364438
15	6	0	2.885757	-1.799747	-0.703579
16	6	0	-2.987327	0.472842	0.096313
17	8	0	-3.431665	1.610038	0.049812
18	6	0	-0.545096	2.292338	-0.019087
19	8	0	-3.814597	-0.622038	0.036907
20	6	0	-5.205611	-0.328217	-0.119534
21	1	0	-1.524915	-1.055090	0.307521
22	1	0	0.595067	-1.601240	-2.420442
23	1	0	0.388510	-3.139109	-1.554211
24	1	0	-0.840912	-1.857927	-1.420461
25	1	0	1.038565	-3.438543	1.141600
26	1	0	1.446008	-2.033302	2.189385
27	1	0	-0.229080	-2.285237	1.627938
28	1	0	3.598606	-1.733150	0.114031
29	1	0	2.843522	-2.805438	-1.137503
30	1	0	3.175178	-1.096180	-1.487090
31	1	0	0.224474	2.699625	-0.678181
32	1	0	-1.538614	2.620689	-0.322215
33	1	0	-0.369306	2.690747	0.989484
34	1	0	-5.695594	-1.292501	-0.268214
35	1	0	-5.606969	0.166203	0.770576
36	1	0	-5.373046	0.321127	-0.983643

TS1₂₂j

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.861079	-1.624299	-2.101167
2	6	0	-1.659435	-1.415542	-0.725850
3	6	0	-2.237055	-2.301984	0.202530
4	6	0	-2.990389	-3.388835	-0.240902
5	6	0	-3.169443	-3.605391	-1.607918
10	8	0	-0.850887	0.990374	-2.706073
11	6	0	-1.741580	1.493756	-0.027287
12	6	0	-1.151744	2.765337	-0.035567
13	6	0	-1.945120	3.898868	0.127027
14	6	0	-3.326304	3.771476	0.295748
15	6	0	-3.913908	2.505980	0.302553
16	6	0	-3.125484	1.365684	0.143916
17	6	0	-0.219186	-0.400556	1.591703
18	6	0	-0.476003	0.488588	2.645397
19	6	0	-0.074363	0.174369	3.944906

20	6	0	0.590248	-1.023648	4.204432
21	6	0	0.852740	-1.914577	3.160972
22	6	0	0.449888	-1.608588	1.862970
23	6	0	2.004773	0.137441	-0.466328
24	6	0	3.141880	0.388239	-1.160754
25	6	0	4.424079	0.100018	-0.522275
26	8	0	4.597738	-0.360897	0.596123
27	1	0	0.975626	1.916458	-2.464176
28	1	0	1.025068	0.214615	-3.099641
29	1	0	2.124675	-0.262952	0.537916
30	1	0	3.151219	0.790099	-2.165861
31	8	0	5.461260	0.413489	-1.351106
32	1	0	-0.988244	1.425162	2.454429
33	1	0	-0.280920	0.870808	4.752551
34	1	0	0.906438	-1.263472	5.215742
35	1	0	1.375843	-2.846245	3.355177
36	1	0	0.655298	-2.311934	1.061206
37	1	0	-3.589902	0.384467	0.138315
38	1	0	-4.988504	2.402966	0.424684
39	1	0	-3.943039	4.657947	0.415601
40	1	0	-1.485620	4.883083	0.109663
41	1	0	-0.081676	2.864386	-0.188484
42	1	0	-2.104454	-2.152709	1.268179
43	1	0	-3.433309	-4.065538	0.484686
44	1	0	-3.751102	-4.457016	-1.951219
45	1	0	-2.756731	-2.878328	-3.595285
46	1	0	-1.467577	-0.880547	-2.793680
47	6	0	6.762618	0.160031	-0.814517
48	1	0	7.466310	0.463231	-1.591623
49	1	0	6.929077	0.740325	0.098044
50	1	0	6.888631	-0.901214	-0.579601

TS1₂₂k

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.815698	-1.730699	0.579759
2	6	0	-2.445827	-0.725625	-0.332919
3	6	0	-3.388020	-0.276396	-1.275964
4	6	0	-4.663089	-0.839690	-1.307090
5	6	0	-5.022698	-1.841057	-0.403789
6	6	0	-4.096910	-2.282007	0.541321
7	15	0	-0.761345	0.015947	-0.226169
8	7	0	0.156922	-0.269496	-1.594590
9	6	0	0.084735	-0.953091	1.086888
10	6	0	0.446815	-2.285517	0.820237
11	6	0	1.076316	-3.054299	1.795399
12	6	0	1.356555	-2.504062	3.049281
13	6	0	1.003033	-1.183729	3.321262
14	6	0	0.368802	-0.409868	2.346098
15	6	0	-0.904728	1.717873	0.412500
16	6	0	-0.061657	2.730440	-0.064468
17	6	0	-0.148024	4.014101	0.471106
18	6	0	-1.081620	4.300252	1.469836
19	6	0	-1.934697	3.298294	1.934230
20	6	0	-1.848397	2.008133	1.408615
21	6	0	1.539374	-0.470365	-1.673058
22	6	0	1.934277	-1.334572	-2.845138
23	6	0	2.428285	0.079188	-0.799052
24	6	0	3.878026	-0.126985	-0.786025
25	8	0	4.569213	-0.808451	-1.527503
26	8	0	4.425735	0.595788	0.237287
27	6	0	5.847778	0.495902	0.356091
28	1	0	-2.115915	-2.088148	1.324933
29	1	0	-3.081984	0.511729	-1.962461
30	1	0	-5.379856	-0.488768	-2.044736
31	1	0	-6.019471	-2.273641	-0.433564

32	1	0	-4.366363	-3.056724	1.254010
33	1	0	0.237538	-2.717515	-0.153581
34	1	0	1.354484	-4.080982	1.574671
35	1	0	1.852235	-3.103523	3.807960
36	1	0	1.223643	-0.747368	4.291393
37	1	0	0.107783	0.618819	2.568556
38	1	0	0.631408	2.520694	-0.869907
39	1	0	0.504904	4.796407	0.094698
40	1	0	-1.150968	5.305044	1.877734
41	1	0	-2.672721	3.518648	2.700580
42	1	0	-2.524003	1.236237	1.766766
43	1	0	3.012048	-1.483706	-2.876181
44	1	0	1.425002	-2.303430	-2.775273
45	1	0	1.605221	-0.872968	-3.784155
46	1	0	2.069563	0.727685	-0.008926
47	1	0	6.117034	1.127707	1.204188
48	1	0	6.153068	-0.538718	0.538979
49	1	0	6.341629	0.848509	-0.554280
50	6	0	-0.680217	0.452227	-2.896417
51	8	0	-1.396664	1.389756	-2.380492
52	1	0	0.167930	0.742363	-3.551068
53	1	0	-1.191250	-0.438512	-3.322213

TS1₂₂l

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.630493	0.041172	2.482744
2	15	0	1.059215	0.778402	0.862118
3	6	0	1.799757	2.387121	1.289970
4	6	0	2.296701	-0.337985	0.106597
5	7	0	-0.380286	0.987506	0.039272
6	6	0	-0.158548	1.899416	-1.385940
7	8	0	1.076312	2.251993	-1.463332
8	6	0	-1.508987	0.241979	0.277846
9	6	0	-2.669390	0.331424	-0.415601
10	6	0	-3.777500	-0.537029	-0.021493
11	8	0	-4.865801	-0.329201	-0.813343
12	6	0	-6.004860	-1.138895	-0.504758
13	8	0	-3.773758	-1.352954	0.888661
14	1	0	-0.552331	1.157998	-2.116236
15	1	0	-0.924838	2.686926	-1.216240
16	1	0	-1.491020	-0.484571	1.088552
17	1	0	-2.820287	1.017612	-1.239173
18	1	0	1.509379	0.054351	3.133462
19	1	0	-0.152248	0.650265	2.942731
20	1	0	0.270101	-0.985855	2.393584
21	1	0	2.758277	2.223528	1.793206
22	1	0	1.918295	2.940965	0.356738
23	1	0	1.115598	2.917464	1.960086
24	1	0	-6.773981	-0.850882	-1.223188
25	1	0	-5.766671	-2.201836	-0.606368
26	1	0	-6.349231	-0.954659	0.517221
27	6	0	2.794590	-1.434997	0.833077
28	6	0	3.737919	-2.286101	0.258357
29	6	0	4.189764	-2.053524	-1.041409
30	6	0	3.695308	-0.967795	-1.766182
31	6	0	2.751435	-0.108730	-1.204158
32	1	0	2.459355	-1.641331	1.843934
33	1	0	4.115450	-3.131117	0.827319
34	1	0	4.923085	-2.719924	-1.487887
35	1	0	4.042401	-0.786645	-2.779747
36	1	0	2.338325	0.744090	-1.744856

TS1₂₂m

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.740419	-0.152921	-1.339689
2	6	0	2.467009	-0.182268	0.038485
3	6	0	3.213760	-1.032035	0.874901
4	6	0	4.221274	-1.835016	0.341144
5	6	0	4.488807	-1.802985	-1.028342
6	6	0	3.748201	-0.963381	-1.861983
7	15	0	1.145921	0.876344	0.745501
8	7	0	-0.384059	0.859954	0.071173
9	6	0	-1.389541	-0.090165	0.254112
10	6	0	-2.662933	0.298030	-0.045887
11	6	0	-3.832103	-0.575793	-0.061564
12	8	0	-3.899070	-1.763660	0.223429
13	6	0	0.923959	0.299514	2.477425
14	6	0	1.739818	2.583747	1.011585
15	6	0	-0.348572	1.816370	-1.314173
16	8	0	0.896095	2.042245	-1.585106
17	8	0	-4.933420	0.132685	-0.449713
18	6	0	-6.150926	-0.616425	-0.499523
19	1	0	-0.942064	1.169753	-1.995092
20	1	0	-0.974324	2.682099	-1.005691
21	6	0	-1.040175	-1.506366	0.658231
22	1	0	-2.851202	1.333524	-0.303928
23	1	0	1.812372	0.542196	3.067845
24	1	0	0.070478	0.837249	2.899738
25	1	0	0.733094	-0.771131	2.546422
26	1	0	2.648066	2.542832	1.622538
27	1	0	1.915754	3.043926	0.041114
28	1	0	0.963517	3.135486	1.551212
29	1	0	-6.919621	0.092846	-0.810709
30	1	0	-6.075967	-1.436645	-1.219758
31	1	0	-6.393086	-1.035704	0.481696
32	1	0	3.023862	-1.078545	1.941929
33	1	0	4.792810	-2.486386	0.996545
34	1	0	5.271790	-2.432440	-1.443007
35	1	0	3.953843	-0.936578	-2.928604
36	1	0	2.151307	0.521790	-1.959025
37	1	0	-1.713499	-2.207114	0.163425
38	1	0	-0.005347	-1.750490	0.401374
39	1	0	-1.185002	-1.663512	1.734038

TS1_{22n}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.615282	-1.130664	-2.028552
2	6	0	2.671096	-0.338173	-1.376429
3	6	0	2.474487	-0.482186	0.007748
4	6	0	3.233047	-1.429914	0.718237
5	6	0	4.177469	-2.213949	0.056165
6	6	0	4.369223	-2.066371	-1.318267
7	15	0	1.238951	0.552291	0.887607
8	6	0	1.925524	2.204324	1.264520
9	7	0	-0.348428	0.612547	0.337613
10	6	0	-0.347352	1.781441	-0.933762
11	8	0	0.900362	1.923391	-1.244828
12	6	0	1.112200	-0.160769	2.580549
13	6	0	-1.273859	-0.429617	0.355941
14	6	0	-0.825993	-1.854454	0.607355
15	6	0	-2.575536	-0.128548	0.067587
16	6	0	-3.663104	-1.090675	-0.071963
17	8	0	-4.817365	-0.432713	-0.395476
18	6	0	-5.966678	-1.267702	-0.558101
19	8	0	-3.637747	-2.306365	0.066677

20	1	0	-1.005296	1.224686	-1.634758
21	6	0	-1.079430	2.996102	-0.392208
22	1	0	-2.864350	0.903172	-0.079745
23	1	0	2.061497	-0.047060	3.112022
24	1	0	0.347491	0.410369	3.115039
25	1	0	0.828097	-1.212640	2.582932
26	1	0	2.575470	2.115381	2.142185
27	1	0	2.466343	2.584083	0.402042
28	1	0	1.099288	2.885336	1.480134
29	1	0	-6.789090	-0.591938	-0.798877
30	1	0	-5.816161	-1.987374	-1.368463
31	1	0	-6.183455	-1.819785	0.361439
32	1	0	3.097583	-1.568770	1.785263
33	1	0	4.759049	-2.941268	0.615811
34	1	0	5.103007	-2.681030	-1.832935
35	1	0	3.760093	-1.014478	-3.099132
36	1	0	2.074507	0.404035	-1.900901
37	1	0	-1.462164	-2.540808	0.048559
38	1	0	0.217243	-2.009718	0.320433
39	1	0	-0.946553	-2.128049	1.662775
40	6	0	-0.559583	4.221151	-0.474301
41	1	0	-2.079632	2.846245	0.011985
42	1	0	-1.098529	5.102064	-0.135217
43	1	0	0.427523	4.360871	-0.906102

TS1₂₂₀

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.624923	-1.954062	-0.562310
2	6	0	-2.356605	-0.606441	-0.269266
3	6	0	-3.173869	0.400069	-0.816768
4	6	0	-4.233447	0.061890	-1.657631
5	6	0	-4.483804	-1.276626	-1.964393
6	6	0	-3.682083	-2.277128	-1.413407
7	15	0	-0.993086	-0.136291	0.864241
8	7	0	0.439932	-0.996837	0.721864
9	6	0	1.615369	-0.512160	0.199839
10	6	0	2.765984	-1.218637	0.083433
11	6	0	3.931871	-0.551923	-0.493474
12	8	0	3.989452	0.599174	-0.899646
13	6	0	-0.606314	1.599946	0.453892
14	6	0	-1.587764	-0.179519	2.586550
15	6	0	0.286350	-2.580970	1.256533
16	8	0	-0.938868	-2.795547	1.598996
17	8	0	5.002603	-1.395025	-0.534507
18	6	0	6.195667	-0.832727	-1.088475
19	1	0	0.687061	-3.110351	0.362572
20	1	0	1.066712	-2.582658	2.050873
21	1	0	1.638677	0.519223	-0.142261
22	1	0	2.870127	-2.249742	0.395007
23	1	0	-2.512175	0.397930	2.683073
24	1	0	-1.738807	-1.239771	2.805995
25	1	0	-0.817368	0.221152	3.251416
26	1	0	6.942388	-1.627506	-1.048312
27	1	0	6.033548	-0.513896	-2.122514
28	1	0	6.527277	0.031764	-0.505501
29	1	0	-2.991223	1.445921	-0.595132
30	1	0	-4.859293	0.846591	-2.073680
31	1	0	-5.306138	-1.537439	-2.625567
32	1	0	-3.882720	-3.321124	-1.638108
33	1	0	-2.028311	-2.715258	-0.060050
34	6	0	-0.535927	2.580353	1.454582
35	6	0	-0.198796	3.895916	1.131964
36	6	0	0.079058	4.244429	-0.189257
37	6	0	0.014198	3.275609	-1.193313
38	6	0	-0.329222	1.963207	-0.877006

39	1	0	-0.743162	2.329117	2.489138
40	1	0	-0.150337	4.645102	1.916897
41	1	0	0.348197	5.267154	-0.437488
42	1	0	0.235184	3.539492	-2.223236
43	1	0	-0.382822	1.220345	-1.667477

TS1₂₂p

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.464954	3.154145	1.554162
2	6	0	1.804174	1.958395	1.273126
3	6	0	1.692310	1.518654	-0.057391
4	6	0	2.251084	2.293189	-1.090750
5	6	0	2.911702	3.485585	-0.796965
6	6	0	3.017512	3.919010	0.525609
7	15	0	0.793754	-0.030894	-0.454333
8	6	0	1.832886	-1.498662	-0.206871
9	7	0	-0.728438	-0.297679	0.163282
10	6	0	-0.505417	-0.830637	1.800357
11	8	0	0.709979	-0.555536	2.104565
12	6	0	0.597183	-0.019331	-2.284440
13	6	0	-1.939845	0.242969	-0.257256
14	6	0	-1.971567	1.542875	-1.032537
15	6	0	-3.073627	-0.405759	0.141955
16	6	0	-4.439072	0.061341	-0.071148
17	8	0	-5.320872	-0.812664	0.500238
18	6	0	-6.700338	-0.465202	0.354123
19	8	0	-4.820586	1.061447	-0.664169
20	1	0	-1.335378	-0.259129	-2.265551
21	1	0	-0.794097	-1.899116	1.702138
22	1	0	-2.980339	-1.347532	0.670224
23	1	0	1.574636	-0.130708	-2.761533
24	1	0	-0.015866	-0.882599	-2.555858
25	1	0	0.115683	0.887913	-2.650297
26	1	0	-7.258021	-1.260788	0.851103
27	1	0	-6.912781	0.499468	0.824756
28	1	0	-6.979887	-0.405890	-0.702150
29	1	0	2.181343	1.979182	-2.126326
30	1	0	3.340597	4.074552	-1.602925
31	1	0	3.529424	4.850654	0.751937
32	1	0	2.546744	3.487632	2.585044
33	1	0	1.375713	1.330895	2.052284
34	1	0	-2.868951	2.106205	-0.775272
35	1	0	-1.084870	2.150255	-0.827699
36	1	0	-2.030715	1.360226	-2.112618
37	6	0	1.276680	-2.764492	-0.439256
38	6	0	2.081764	-3.900711	-0.366616
39	6	0	3.442553	-3.780286	-0.079277
40	6	0	3.997216	-2.518170	0.141556
41	6	0	3.198136	-1.377571	0.078686
42	1	0	0.215915	-2.863411	-0.651091
43	1	0	1.643286	-4.880649	-0.533954
44	1	0	4.067958	-4.667061	-0.024936
45	1	0	5.054180	-2.419627	0.373011
46	1	0	3.630282	-0.401316	0.273150

TS1₄₂a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.477750	-0.891319	0.638924
2	15	0	-1.545199	0.180717	0.154237

3	7	0	-0.710267	-1.048301	-0.468829
4	6	0	0.568273	-1.378568	-0.290620
5	1	0	1.132297	-0.448963	1.568261
6	1	0	2.467268	-1.339369	0.672667
7	1	0	-2.825959	-0.370153	0.400619
8	1	0	-1.277148	0.792182	1.396588
9	1	0	-1.899576	1.236288	-0.702521
10	1	0	0.950942	-2.056612	-1.059907
11	6	0	1.584219	1.033570	-0.256537
12	8	0	0.433570	1.525075	-0.132325
13	1	0	1.962416	0.715069	-1.244213
14	1	0	2.389613	1.316210	0.444738

TS1₄₂gb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.275068	1.557442	-0.390634
2	8	0	-0.980317	1.542084	-0.185750
3	6	0	0.990178	-0.080506	0.575799
4	6	0	2.456241	-0.044205	0.556405
5	1	0	2.928403	0.433800	1.443219
6	6	0	0.334735	-0.998398	-0.290042
7	7	0	-0.949037	-1.209204	-0.439664
8	15	0	-2.185119	-0.331097	0.189581
9	1	0	0.513799	0.194465	1.514290
10	1	0	-3.096170	-1.366284	0.517715
11	1	0	-2.175959	0.372657	1.408047
12	1	0	-2.974111	0.384368	-0.719657
13	1	0	0.980153	-1.539153	-0.987499
14	1	0	0.686924	1.319970	-1.385808
15	1	0	0.892709	2.283125	0.164399
16	8	0	3.146188	-0.449342	-0.367992

TS1₄₂c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.088847	-1.050959	0.491013
2	6	0	-1.168504	-1.503319	-0.481658
3	7	0	0.068136	-1.116440	-0.717681
4	15	0	1.041553	-0.021627	-0.006014
5	6	0	2.657501	-0.872451	0.145584
6	6	0	0.714822	0.653274	1.664486
7	6	0	1.325347	1.379009	-1.131525
8	1	0	-3.009474	-1.630089	0.560233
9	1	0	-1.702534	-0.742004	1.458753
10	1	0	-1.565304	-2.172198	-1.253547
11	1	0	3.433679	-0.179462	0.486197
12	1	0	2.940307	-1.284715	-0.826612
13	1	0	2.575745	-1.696535	0.861029
14	1	0	0.586268	-0.163440	2.381518
15	1	0	-0.196533	1.253211	1.588352
16	1	0	1.565052	1.269397	1.978289
17	1	0	0.366248	1.896117	-1.218437
18	1	0	1.637556	0.993286	-2.106152
19	1	0	2.098256	2.046040	-0.735051

20	6	0	-2.526664	0.685510	-0.147728
21	8	0	-1.500992	1.443064	-0.095252
22	1	0	-2.964379	0.433154	-1.137214
23	1	0	-3.339127	0.825825	0.597593

TS1_{42d}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.716558	-0.082560	0.463853
2	6	0	-1.009182	-0.965420	-0.457241
3	7	0	0.261288	-1.030574	-0.672114
4	15	0	1.516743	-0.159082	0.006951
5	6	0	-3.183541	-0.296430	0.532736
6	6	0	2.708150	-1.554126	0.237424
7	6	0	1.548847	0.585242	1.688132
8	6	0	2.377690	0.872037	-1.225652
9	8	0	-3.855072	-0.738598	-0.383831
10	1	0	-1.259565	0.035585	1.447189
11	1	0	-1.639494	-1.550432	-1.133665
12	1	0	-3.669702	0.040074	1.475580
13	1	0	3.681553	-1.188283	0.580827
14	1	0	2.837013	-2.089949	-0.706659
15	1	0	2.317459	-2.259465	0.978362
16	1	0	0.985494	-0.055306	2.374566
17	1	0	1.097167	1.573565	1.643493
18	1	0	2.588458	0.620829	2.032847
19	1	0	2.420666	0.307325	-2.161704
20	1	0	3.398424	1.075771	-0.885245
21	1	0	1.809797	1.789913	-1.365001
22	6	0	-1.368041	1.476021	-0.243837
23	8	0	-0.075825	1.682645	-0.217839
24	1	0	-1.858431	1.400993	-1.237447
25	1	0	-1.986013	2.138675	0.398266

TS1_{42e}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.318504	-1.019082	0.576851
2	15	0	1.821558	-0.068521	0.033663
3	6	0	2.504389	0.863959	-1.379841
4	7	0	0.908187	-1.402200	-0.432223
5	6	0	-0.345159	-1.624432	-0.242415
6	6	0	-1.323150	-0.762341	0.428147
7	6	0	-1.307143	0.637672	-0.640057
8	8	0	-0.084442	1.120684	-0.650020
9	6	0	-2.676004	-1.367741	0.542644
10	8	0	-3.136352	-2.161954	-0.260598
11	6	0	1.559476	0.960952	1.535412
12	1	0	-0.988275	-0.305014	1.359892
13	1	0	-0.756716	-2.507470	-0.740674
14	1	0	-3.288910	-1.015197	1.400202
15	1	0	4.135487	-0.346709	0.859779
16	1	0	3.655189	-1.670692	-0.234010
17	1	0	3.070596	-1.650504	1.436584
18	1	0	1.212581	0.316359	2.350054

19	1	0	0.824789	1.733889	1.327978
20	1	0	2.523309	1.389486	1.832118
21	1	0	2.610083	0.161843	-2.212443
22	1	0	3.493495	1.252263	-1.116629
23	1	0	1.816178	1.659140	-1.656318
24	1	0	-1.657282	0.173446	-1.588681
25	6	0	-2.396935	1.549357	-0.120442
26	6	0	-2.169887	2.793537	0.300764
27	1	0	-3.411990	1.150660	-0.149874
28	1	0	-2.974030	3.439763	0.642101
29	1	0	-1.163376	3.200821	0.289093

TS1₄₂f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.330908	-1.577836	0.556613
2	15	0	2.203935	-0.177945	0.136298
3	6	0	3.258768	0.886977	-0.899110
4	7	0	1.083103	-1.004571	-0.775616
5	6	0	-0.208122	-0.940610	-0.788402
6	6	0	-1.064972	-0.075011	0.003931
7	6	0	-0.621375	1.510350	-0.602173
8	8	0	0.645085	1.727768	-0.367990
9	6	0	-2.519545	-0.325264	-0.189348
10	8	0	-3.032751	-0.765766	-1.201521
11	6	0	1.910216	0.554677	1.794608
12	1	0	-0.796152	0.031595	1.052932
13	1	0	-0.703629	-1.505180	-1.583612
14	8	0	-3.235053	0.069599	0.894018
15	1	0	4.234447	-1.218488	1.060166
16	1	0	3.613584	-2.107627	-0.356754
17	1	0	2.817252	-2.284003	1.217105
18	1	0	1.262269	-0.111054	2.373950
19	1	0	1.433630	1.523846	1.660625
20	1	0	2.871198	0.635722	2.315223
21	1	0	3.526586	0.326409	-1.799591
22	1	0	4.172093	1.144788	-0.352457
23	1	0	2.683676	1.774243	-1.160287
24	1	0	-0.948310	1.468451	-1.663566
25	1	0	-1.349591	2.127073	-0.035005
26	6	0	-4.658777	-0.053288	0.762805
27	1	0	-5.073067	0.319214	1.700515
28	1	0	-5.021814	0.540890	-0.080250
29	1	0	-4.943776	-1.097488	0.606250

TS1₄₂g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.233897	0.189654	0.948150
2	6	0	-0.009465	0.366616	1.717812
3	7	0	1.209138	0.188141	1.353272
4	15	0	2.012373	-0.169091	-0.068368
5	6	0	-1.468997	-1.164680	0.382021
6	6	0	3.265399	-1.336786	0.617327
7	6	0	2.965987	1.335531	-0.460135

8	6	0	1.590362	-1.027031	-1.640032
9	8	0	-0.634765	-2.028891	0.167505
10	8	0	-2.783390	-1.337540	0.098490
11	6	0	-3.123881	-2.581489	-0.529749
12	1	0	-2.117229	0.528378	1.488977
13	1	0	-0.121477	0.816759	2.711748
14	1	0	4.075897	-1.499680	-0.100779
15	1	0	2.782961	-2.298302	0.821768
16	1	0	3.678008	-0.946983	1.550503
17	1	0	3.445581	1.698236	0.453095
18	1	0	2.259221	2.073925	-0.839581
19	1	0	3.729872	1.113508	-1.211860
20	1	0	1.148243	-0.307943	-2.324529
21	1	0	0.872664	-1.819402	-1.430504
22	1	0	2.518482	-1.458226	-2.033445
23	1	0	-4.210031	-2.570961	-0.628439
24	1	0	-2.801194	-3.428258	0.081536
25	1	0	-2.653759	-2.655172	-1.514823
26	6	0	-1.037867	1.278379	-0.475278
27	8	0	0.138383	1.104502	-1.015828
28	6	0	-1.301243	2.699675	-0.029055
29	6	0	-2.446882	3.354074	-0.223861
30	1	0	-1.914150	0.901826	-1.043458
31	1	0	-0.424650	3.216615	0.363194
32	1	0	-2.559930	4.408265	0.016499
33	1	0	-3.316989	2.858575	-0.651827

TS1₄₂h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.315123	0.388313	-1.651497
2	15	0	2.235339	-0.142898	-0.254374
3	6	0	1.898041	-1.892558	-0.702351
4	6	0	3.345814	-0.052387	1.186561
5	7	0	1.145711	1.097639	-0.242151
6	6	0	-0.149340	1.162611	-0.130081
7	6	0	-0.992356	-0.026728	-0.017744
8	6	0	-2.469319	0.112203	-0.090777
9	8	0	-3.145387	1.016483	0.365796
10	6	0	-0.720634	2.547785	0.048991
11	8	0	-3.019995	-0.987731	-0.674470
12	6	0	-4.453575	-1.012226	-0.695078
13	1	0	4.199473	-0.252479	-1.732055
14	1	0	3.631813	1.422963	-1.496673
15	1	0	2.757216	0.337240	-2.592148
16	1	0	1.262430	-1.931101	-1.592735
17	1	0	1.404408	-2.367784	0.143789
18	1	0	2.852123	-2.377122	-0.940295
19	1	0	3.672117	0.985140	1.302288
20	1	0	4.221249	-0.689332	1.020747
21	1	0	2.780330	-0.373171	2.060823
22	1	0	-0.654882	-0.855000	-0.635966
23	1	0	-1.204583	2.631370	1.027639
24	1	0	0.081599	3.283088	-0.034515
25	1	0	-1.502202	2.753765	-0.689040
26	1	0	-4.724100	-1.953411	-1.175722
27	1	0	-4.856932	-0.970836	0.320547
28	1	0	-4.847820	-0.165251	-1.263910

29	6	0	-0.561951	-0.642321	1.593236
30	8	0	0.705176	-0.929562	1.639125
31	1	0	-1.276994	-1.491688	1.643556
32	1	0	-0.934479	0.171948	2.253187

TS1_{42i}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.511964	-1.245625	1.259985
2	15	0	2.357542	-0.150695	0.320928
3	6	0	1.916963	1.062522	1.630019
4	6	0	3.461665	0.578432	-0.933996
5	7	0	1.361202	-1.310625	-0.321072
6	6	0	0.070516	-1.381713	-0.446424
7	6	0	-0.839114	-0.342939	0.053808
8	6	0	-2.297204	-0.635766	0.068011
9	8	0	-2.947319	-1.123398	-0.839726
10	6	0	-0.467894	1.024860	-1.052657
11	6	0	-1.447927	2.111155	-0.661283
12	6	0	-1.058899	3.331789	-0.291900
13	8	0	0.802724	1.300586	-0.945438
14	1	0	-0.526603	0.080672	1.004686
15	6	0	-0.445082	-2.530444	-1.278551
16	8	0	-2.864994	-0.218693	1.231266
17	1	0	4.338494	-0.670380	1.690467
18	1	0	3.915610	-2.012165	0.593304
19	1	0	2.972992	-1.746703	2.070566
20	1	0	1.367286	0.553030	2.428156
21	1	0	1.316024	1.859081	1.197786
22	1	0	2.847352	1.455599	2.056260
23	1	0	3.795447	-0.226741	-1.595053
24	1	0	4.333705	1.018637	-0.439023
25	1	0	2.903160	1.321202	-1.500292
26	1	0	-0.802497	0.578013	-2.016725
27	1	0	-2.507325	1.872132	-0.754831
28	1	0	-1.771559	4.115226	-0.048214
29	1	0	-0.001392	3.576014	-0.249504
30	6	0	-4.289422	-0.367780	1.302673
31	1	0	-4.574946	0.011593	2.284704
32	1	0	-4.780280	0.208180	0.512877
33	1	0	-4.575531	-1.418332	1.199467
34	1	0	-0.970917	-2.150271	-2.160212
35	1	0	0.392036	-3.160605	-1.583649
36	1	0	-1.179283	-3.124304	-0.724124

TS1_{42j}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.556465	-2.001644	-0.123796
2	6	0	1.777828	-1.166584	-0.943162
3	6	0	1.948176	-1.246034	-2.334458
4	6	0	2.864874	-2.140595	-2.888729
5	6	0	3.632227	-2.964033	-2.064552
6	6	0	3.475873	-2.891504	-0.679456
7	15	0	0.611368	0.095503	-0.232619

8	7	0	-0.304845	0.420359	-1.578849
9	6	0	-1.594519	0.454428	-1.721137
10	6	0	-2.574371	0.245939	-0.691542
11	6	0	-3.986353	0.316008	-1.132661
12	8	0	-4.398217	0.905337	-2.116076
13	6	0	0.004629	-0.761023	1.275173
14	6	0	-0.365311	-2.112582	1.188184
15	6	0	-0.836088	-2.788150	2.315424
16	6	0	-0.915527	-2.127705	3.541721
17	6	0	-0.540336	-0.784927	3.634899
18	6	0	-0.096211	-0.096394	2.507143
19	6	0	1.741526	1.480147	0.143230
20	6	0	1.546688	2.726168	-0.464913
21	6	0	2.450956	3.760712	-0.229911
22	6	0	3.540250	3.566478	0.621728
23	6	0	3.730883	2.327948	1.235629
24	6	0	2.840285	1.282576	0.989191
25	6	0	-2.205578	1.663620	0.444235
26	8	0	-0.926916	1.817637	0.569523
27	8	0	-4.806684	-0.318898	-0.254378
28	1	0	-1.959472	0.819705	-2.685034
29	1	0	-2.374215	-0.564013	0.003355
30	1	0	1.353361	-0.607023	-2.977089
31	1	0	2.978112	-2.191627	-3.968390
32	1	0	4.346211	-3.659485	-2.497737
33	1	0	4.064989	-3.531928	-0.028377
34	1	0	2.436621	-1.977378	0.954879
35	1	0	0.677216	2.879117	-1.090758
36	1	0	2.295747	4.725447	-0.705068
37	1	0	4.238336	4.378473	0.807439
38	1	0	4.575247	2.169956	1.900973
39	1	0	3.009475	0.319147	1.460072
40	1	0	0.136078	0.959788	2.560072
41	1	0	-0.608575	-0.265285	4.586688
42	1	0	-1.274423	-2.655252	4.421426
43	1	0	-1.133358	-3.829882	2.233150
44	1	0	-0.286779	-2.642340	0.243319
45	1	0	-2.775601	1.274635	1.310711
46	1	0	-2.763382	2.481731	-0.050581
47	6	0	-6.205022	-0.242654	-0.562772
48	1	0	-6.712843	-0.776796	0.241530
49	1	0	-6.537647	0.798395	-0.601656
50	1	0	-6.415237	-0.714223	-1.527056

TS1₄₂k

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.923440	0.956896	-1.315428
2	6	0	-1.830281	1.353357	-0.534514
3	6	0	-1.651951	2.707183	-0.225980
4	6	0	-2.565059	3.651312	-0.692743
5	6	0	-3.649424	3.256464	-1.478827
6	6	0	-3.824811	1.908506	-1.793924
7	15	0	-0.681191	0.106406	0.147236
8	6	0	-0.098079	-1.072737	-1.139255
9	6	0	0.278227	-2.369655	-0.754092
10	6	0	0.737010	-3.282386	-1.704963
11	6	0	0.800589	-2.915800	-3.049605

12	6	0	0.420545	-1.629054	-3.439036
13	6	0	-0.013858	-0.703985	-2.490575
14	6	0	-1.821410	-0.963445	1.152146
15	6	0	-2.612237	-1.963201	0.561024
16	6	0	-3.512268	-2.706137	1.325085
17	6	0	-3.636689	-2.463981	2.694110
18	6	0	-2.857159	-1.473956	3.292606
19	6	0	-1.959698	-0.726496	2.528521
20	7	0	0.248320	0.757016	1.344114
21	6	0	1.539735	0.884196	1.499476
22	6	0	2.479172	0.369667	0.529099
23	6	0	3.935433	0.429589	0.769693
24	8	0	4.571110	-0.531533	0.040452
25	6	0	6.001398	-0.509426	0.120727
26	8	0	4.545044	1.240482	1.445930
27	6	0	2.104856	1.461859	-0.955707
28	8	0	0.833611	1.632101	-1.076000
29	6	0	1.979035	1.753989	2.651559
30	1	0	2.182556	-0.573828	0.083374
31	1	0	-1.355713	0.044069	2.993851
32	1	0	-2.946006	-1.279451	4.358160
33	1	0	-4.335670	-3.044970	3.289895
34	1	0	-4.111516	-3.478235	0.849846
35	1	0	-2.516441	-2.182954	-0.497731
36	1	0	-0.786750	3.007868	0.350399
37	1	0	-2.420901	4.700787	-0.450857
38	1	0	-4.354797	3.997169	-1.846209
39	1	0	-4.664570	1.593413	-2.407272
40	1	0	-3.079535	-0.089663	-1.558269
41	1	0	-0.250696	0.312923	-2.777243
42	1	0	0.476710	-1.337734	-4.484322
43	1	0	1.151445	-3.628179	-3.791560
44	1	0	1.038568	-4.278498	-1.393185
45	1	0	0.213835	-2.671775	0.287129
46	1	0	2.627742	0.823678	-1.694957
47	1	0	2.714633	2.350746	-0.701089
48	1	0	6.344555	-1.316718	-0.528070
49	1	0	6.395860	0.451320	-0.222234
50	1	0	6.335954	-0.677826	1.148581
51	1	0	2.720007	1.246364	3.276037
52	1	0	2.475477	2.653656	2.271758
53	1	0	1.108933	2.037666	3.247207

TS1₄₂l

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.519156	-0.160919	0.027770
2	15	0	0.960885	0.843888	-0.085610
3	6	0	0.653204	1.196748	1.692777
4	6	0	1.523229	2.311464	-1.013303
5	7	0	0.047907	-0.174895	-1.039406
6	6	0	-1.193832	-0.516859	-0.956207
7	6	0	-2.176833	-0.062338	0.019952
8	6	0	-3.507220	-0.721614	-0.125144
9	8	0	-4.182980	-0.731563	1.049993
10	6	0	-5.510540	-1.274243	0.986361
11	6	0	-2.276230	1.618652	-0.338395
12	8	0	-1.099378	2.176674	-0.167171

13	8	0	-3.972017	-1.148432	-1.165662
14	1	0	-1.837554	-0.045299	1.054324
15	1	0	-1.586150	-1.099175	-1.795185
16	1	0	0.277838	0.285916	2.170093
17	1	0	-0.083781	1.993744	1.761001
18	1	0	1.599152	1.461085	2.175054
19	1	0	1.819607	1.974568	-2.010704
20	1	0	2.392460	2.754460	-0.518250
21	1	0	0.691330	3.011096	-1.073046
22	1	0	-2.701919	1.640591	-1.365052
23	1	0	-3.073860	1.924651	0.370389
24	1	0	-5.909009	-1.193519	1.998367
25	1	0	-6.126533	-0.705845	0.284271
26	1	0	-5.484947	-2.319671	0.666556
27	6	0	2.594381	-1.454688	-0.505510
28	6	0	3.769419	-2.201938	-0.399004
29	6	0	4.889656	-1.664382	0.234131
30	6	0	4.831314	-0.373241	0.763011
31	6	0	3.655794	0.369606	0.661399
32	1	0	1.729623	-1.867772	-1.012767
33	1	0	3.808048	-3.204283	-0.817187
34	1	0	5.804743	-2.245084	0.313544
35	1	0	5.700427	0.055935	1.254346
36	1	0	3.637917	1.373627	1.079943

TS1_{42m}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.588447	-0.115823	-0.112545
2	15	0	-1.051324	0.896944	0.106398
3	6	0	-0.728460	1.417204	-1.628337
4	6	0	-1.628207	2.292108	1.130606
5	7	0	-0.129138	-0.148251	0.996810
6	6	0	1.120393	-0.502998	0.957579
7	6	0	2.052402	0.006531	-0.054779
8	6	0	3.414057	-0.588623	-0.152524
9	8	0	3.827368	-0.615860	-1.447850
10	6	0	5.175253	-1.064060	-1.647969
11	6	0	2.202528	1.686601	0.377755
12	8	0	1.034690	2.272532	0.332155
13	8	0	4.128232	-0.936376	0.769965
14	1	0	1.603590	0.082614	-1.042688
15	6	0	1.605514	-1.335222	2.118687
16	1	0	-0.376815	0.553552	-2.201460
17	1	0	0.026115	2.201279	-1.609988
18	1	0	-1.666534	1.758251	-2.077529
19	1	0	-1.976834	1.883711	2.083153
20	1	0	-2.460530	2.803109	0.637105
21	1	0	-0.781126	2.959918	1.281641
22	1	0	2.711447	1.637213	1.365977
23	1	0	2.951725	2.006720	-0.378715
24	1	0	5.345390	-1.010197	-2.724035
25	1	0	5.880441	-0.419999	-1.115359
26	1	0	5.299005	-2.090717	-1.291761
27	1	0	2.374484	-0.790597	2.676222
28	1	0	0.764953	-1.568817	2.774700
29	1	0	2.084637	-2.256866	1.773020
30	6	0	-2.638560	-1.456618	0.290829

31	6	0	-3.796205	-2.214173	0.101115
32	6	0	-4.923436	-1.639956	-0.486033
33	6	0	-4.889711	-0.302110	-0.884965
34	6	0	-3.731124	0.451566	-0.701076
35	1	0	-1.767829	-1.898702	0.762589
36	1	0	-3.816280	-3.253552	0.417936
37	1	0	-5.825133	-2.229033	-0.630359
38	1	0	-5.764667	0.154942	-1.339368
39	1	0	-3.730524	1.491847	-1.018915

TS1_{42n}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.852090	-0.058867	-0.116094
2	15	0	-1.228152	0.761806	0.264948
3	7	0	-0.455076	-0.496416	1.025395
4	6	0	0.758962	-0.944747	0.947691
5	6	0	1.140625	-1.996798	1.959707
6	6	0	-0.810777	1.419297	-1.401628
7	6	0	-1.736302	2.064846	1.439350
8	6	0	1.766438	-0.369946	0.037151
9	6	0	2.039304	1.211877	0.741006
10	8	0	0.896148	1.856861	0.765606
11	6	0	3.047445	-1.115231	-0.134724
12	8	0	3.386295	-1.199521	-1.447218
13	6	0	4.656413	-1.811204	-1.712992
14	8	0	3.754948	-1.550743	0.755606
15	6	0	3.154996	1.832197	-0.078298
16	6	0	3.030781	3.006747	-0.696197
17	1	0	1.354236	-0.109428	-0.934919
18	1	0	-0.672412	0.578516	-2.088708
19	1	0	0.089302	2.024838	-1.333011
20	1	0	-1.657469	2.010666	-1.764688
21	1	0	-2.054287	1.564626	2.358592
22	1	0	-2.584649	2.622140	1.031384
23	1	0	-0.880825	2.708464	1.633590
24	1	0	2.462587	0.926598	1.732217
25	1	0	4.105136	1.297570	-0.092647
26	1	0	3.851082	3.455070	-1.250583
27	1	0	2.096887	3.557851	-0.635708
28	1	0	4.767960	-1.794764	-2.797817
29	1	0	5.464430	-1.248608	-1.236681
30	1	0	4.677266	-2.839180	-1.340477
31	1	0	1.954554	-1.632021	2.594323
32	1	0	0.271550	-2.245421	2.571289
33	1	0	1.523753	-2.897917	1.468703
34	6	0	-3.903040	0.684767	-0.679523
35	6	0	-5.121062	0.082161	-0.991717
36	6	0	-5.309062	-1.279900	-0.748216
37	6	0	-4.275356	-2.029263	-0.187158
38	6	0	-3.057837	-1.422989	0.129889
39	1	0	-3.783128	1.747317	-0.879244
40	1	0	-5.921649	0.675668	-1.425071
41	1	0	-6.257017	-1.751691	-0.992592
42	1	0	-4.415100	-3.088978	0.009419
43	1	0	-2.260153	-2.003959	0.579204

TS1₄₂o

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.937613	1.486404	0.901146
2	6	0	-1.757242	1.475815	0.139315
3	6	0	-1.481536	2.568850	-0.691904
4	6	0	-2.360903	3.652673	-0.753995
5	6	0	-3.527451	3.654766	0.009946
6	6	0	-3.816251	2.566482	0.837151
7	15	0	-0.564091	0.065918	0.303281
8	7	0	0.456139	0.414422	-0.963010
9	6	0	1.746277	0.415435	-1.044974
10	6	0	2.705845	0.087949	-0.006340
11	6	0	2.359020	-1.615648	0.240643
12	8	0	1.136099	-1.747875	0.677010
13	6	0	-0.137095	0.233623	2.085107
14	6	0	-1.618022	-1.380533	-0.038098
15	6	0	4.124605	0.285640	-0.410202
16	8	0	4.553241	0.206772	-1.546900
17	8	0	4.918145	0.500633	0.669119
18	6	0	6.319390	0.618011	0.382291
19	1	0	2.492330	0.480792	0.985570
20	1	0	2.158490	0.544947	-2.050092
21	1	0	0.396366	1.181043	2.215042
22	1	0	0.486170	-0.604011	2.387920
23	1	0	-1.065326	0.288075	2.662115
24	1	0	2.605744	-2.061797	-0.746115
25	1	0	3.171752	-1.864841	0.954285
26	1	0	6.805051	0.765362	1.347718
27	1	0	6.692312	-0.289222	-0.100861
28	1	0	6.508805	1.470608	-0.275932
29	1	0	-0.582010	2.560850	-1.297977
30	1	0	-2.133410	4.492687	-1.404887
31	1	0	-4.212347	4.496991	-0.040903
32	1	0	-4.727560	2.557087	1.429053
33	1	0	-3.186677	0.639162	1.535744
34	6	0	-1.541093	-2.554801	0.725147
35	6	0	-2.396231	-3.619749	0.443574
36	6	0	-3.309480	-3.534225	-0.609104
37	6	0	-3.372994	-2.374946	-1.383782
38	6	0	-2.537980	-1.296459	-1.094400
39	1	0	-0.789254	-2.644714	1.497805
40	1	0	-2.335538	-4.525841	1.040122
41	1	0	-3.966950	-4.371372	-0.828619
42	1	0	-4.075404	-2.305421	-2.209751
43	1	0	-2.601507	-0.392076	-1.691352

TS1₄₂p

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.609324	0.206657	-0.029915
2	6	0	-2.514057	-0.672690	-0.065660
3	6	0	-2.641311	-1.883148	-0.758826
4	6	0	-3.834909	-2.204512	-1.409668
5	6	0	-4.916670	-1.325477	-1.367358
6	6	0	-4.802070	-0.117776	-0.674111

7	15	0	-0.961779	-0.258422	0.853782
8	7	0	-0.033216	-1.581328	0.533758
9	6	0	1.216921	-1.736700	0.186590
10	6	0	1.728201	-3.156033	0.211386
11	6	0	-0.615860	1.444998	0.249842
12	6	0	-1.564436	-0.266130	2.579154
13	6	0	2.100854	-0.612939	-0.040496
14	6	0	2.292724	0.062951	1.678335
15	8	0	1.138868	0.166519	2.243716
16	6	0	3.457755	-0.817356	-0.591758
17	8	0	4.174618	-1.793880	-0.455535
18	8	0	3.877835	0.308095	-1.235817
19	6	0	5.222711	0.261138	-1.727867
20	1	0	1.611521	0.248305	-0.484910
21	1	0	-1.979069	-1.260445	2.767488
22	1	0	-2.360332	0.476080	2.690761
23	1	0	-0.732406	-0.068395	3.251524
24	1	0	3.011264	-0.668058	2.102271
25	1	0	2.821145	0.991510	1.379659
26	1	0	5.401572	1.234613	-2.186866
27	1	0	5.929815	0.086506	-0.911976
28	1	0	5.338388	-0.536450	-2.467603
29	1	0	2.494665	-3.262294	0.986913
30	1	0	0.900602	-3.837462	0.418201
31	1	0	2.217950	-3.421621	-0.730022
32	1	0	-1.802631	-2.570532	-0.778058
33	1	0	-3.917551	-3.145699	-1.946695
34	1	0	-5.845893	-1.577975	-1.871192
35	1	0	-5.640228	0.572952	-0.637991
36	1	0	-3.530430	1.157973	0.490350
37	6	0	-0.130727	2.452481	1.099040
38	6	0	0.074294	3.740521	0.605923
39	6	0	-0.172585	4.031628	-0.737576
40	6	0	-0.636124	3.030144	-1.591367
41	6	0	-0.870278	1.746052	-1.098706
42	1	0	0.133496	2.199321	2.118201
43	1	0	0.443728	4.515529	1.271970
44	1	0	0.001427	5.034307	-1.119040
45	1	0	-0.824213	3.246765	-2.639306
46	1	0	-1.254840	0.981982	-1.767391

INT_{22a}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.316040	-0.080855	0.000549
2	6	0	1.585850	-0.636908	-0.000058
3	6	0	2.738860	0.044446	-0.000158
4	6	0	-0.108213	1.317152	0.000162
5	15	0	-1.272353	-0.719959	0.000033
6	8	0	-1.487756	1.038919	-0.000476
7	1	0	1.572260	-1.724813	-0.000471
8	1	0	2.777965	1.129401	0.000338
9	1	0	3.682359	-0.488346	-0.000721
10	1	0	0.225068	1.856391	-0.899609
11	1	0	0.224181	1.856632	0.900114
12	1	0	-2.109535	-0.921952	-1.123219
13	1	0	-2.108380	-0.922080	1.124000
14	1	0	-0.787845	-2.079349	-0.000636

INT_{22b}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.803365	0.745444	0.000011
2	6	0	0.803189	-0.170455	-0.000033
3	7	0	-0.533437	0.087038	-0.000059
4	15	0	-1.951605	-0.915381	0.000014
5	8	0	-2.551097	0.747889	-0.000047
6	6	0	-1.279507	1.347516	0.000027
7	6	0	3.192489	0.291400	0.000018
8	8	0	3.553690	-0.877643	-0.000014
9	1	0	1.607082	1.814238	0.000035
10	1	0	1.065600	-1.227236	-0.000064
11	1	0	-2.713574	-1.299054	-1.126680
12	1	0	-2.713184	-1.298930	1.127011
13	1	0	-1.157049	-2.114963	0.000011
14	1	0	-1.082895	1.947049	-0.900447
15	1	0	-1.082906	1.946871	0.900625
16	1	0	3.947101	1.108085	0.000057

INT_{22c}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.377274	-0.257754	0.134862
2	6	0	2.116209	-0.674891	-0.091978
3	7	0	1.001006	0.096442	-0.310638
4	15	0	-0.856190	-0.076331	-0.001934
5	8	0	-0.493910	1.582238	0.009216
6	6	0	0.935339	1.511856	-0.119152
7	6	0	-2.671055	0.389025	0.179414
8	6	0	-1.071867	-1.185834	-1.462803
9	6	0	-0.712836	-1.076502	1.541783
10	1	0	4.175861	-0.979395	0.263092
11	1	0	3.647280	0.793744	0.168122
12	1	0	1.913968	-1.745866	-0.144302
13	1	0	1.268128	2.115518	-0.975486
14	1	0	1.426417	1.874762	0.798776
15	1	0	-2.823376	1.005187	1.070952
16	1	0	-3.296119	-0.507242	0.257919
17	1	0	-3.002739	0.970173	-0.687396
18	1	0	-2.027389	-1.717894	-1.429073
19	1	0	-0.243371	-1.894712	-1.531901
20	1	0	-1.050612	-0.561116	-2.362518
21	1	0	-1.643041	-1.611707	1.753969
22	1	0	-0.516452	-0.384535	2.368445
23	1	0	0.120162	-1.780352	1.486395

INT_{22d}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.687774	0.723951	-0.000006
2	6	0	1.526284	-0.004174	0.000049
3	7	0	0.262923	0.439991	0.000085
4	15	0	-1.576992	-0.190239	0.000000
5	8	0	-1.591668	1.497126	-0.000033
6	6	0	-0.186391	1.797834	0.000010
7	6	0	3.961665	0.035429	-0.000028
8	6	0	-3.448385	-0.176230	-0.000087
9	6	0	-1.324210	-1.197259	-1.519445
10	6	0	-1.324348	-1.197225	1.519490

11	8	0	4.124542	-1.183484	-0.000005
12	1	0	2.683022	1.811167	-0.000030
13	1	0	1.637240	-1.089442	0.000076
14	1	0	0.081207	2.371550	-0.898747
15	1	0	0.081135	2.371631	0.898737
16	1	0	4.849274	0.708822	-0.000071
17	1	0	-3.828285	0.344847	0.884215
18	1	0	-3.839605	-1.199349	-0.000087
19	1	0	-3.828203	0.344816	-0.884442
20	1	0	-2.127554	-1.929376	-1.643258
21	1	0	-0.354635	-1.699171	-1.499118
22	1	0	-1.336910	-0.518259	-2.379041
23	1	0	-2.127699	-1.929346	1.643242
24	1	0	-1.337136	-0.518205	2.379069
25	1	0	-0.354766	-1.699128	1.499267

INT_{22e}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.402638	-0.412684	0.000954
2	6	0	3.800548	-0.050487	-0.021378
3	8	0	4.743454	-0.811955	0.156441
4	6	0	1.445716	0.543082	-0.215038
5	7	0	0.110954	0.387241	-0.225044
6	6	0	-0.871114	1.409386	-0.498052
7	8	0	-2.014080	0.542626	-0.320559
8	15	0	-1.283367	-0.942047	0.010444
9	6	0	-0.889256	2.568332	0.452131
10	6	0	-2.985660	-1.713854	0.140502
11	6	0	-0.670627	-1.424714	1.676627
12	6	0	-0.614806	-2.021695	-1.319200
13	6	0	-0.761799	3.835918	0.059797
14	1	0	2.159729	-1.454331	0.191294
15	1	0	3.985915	1.034085	-0.224209
16	1	0	1.790853	1.565807	-0.395764
17	1	0	-0.856263	1.769484	-1.537823
18	1	0	-0.975764	2.309850	1.506603
19	1	0	-2.908777	-2.782249	0.369685
20	1	0	-3.566765	-1.227450	0.930255
21	1	0	-3.533998	-1.595097	-0.799188
22	1	0	-1.105413	-0.730785	2.404802
23	1	0	0.416671	-1.351845	1.738230
24	1	0	-1.001659	-2.436377	1.929627
25	1	0	-0.960020	-3.052096	-1.192374
26	1	0	0.475787	-1.985353	-1.350237
27	1	0	-0.999290	-1.646399	-2.274397
28	1	0	-0.743025	4.658063	0.769249
29	1	0	-0.672989	4.099625	-0.992222

INT_{22f}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.859355	0.558024	0.000237
2	6	0	-0.675158	-0.119862	0.000550
3	7	0	0.569505	0.387601	0.000676
4	15	0	2.420417	-0.158008	-0.000075
5	8	0	2.368186	1.530726	-0.000432
6	6	0	0.950363	1.765416	0.000126
7	6	0	-3.101047	-0.196561	0.000121
8	6	0	4.291764	-0.061644	-0.000973
9	6	0	2.221837	-1.179950	1.518680
10	6	0	2.220438	-1.180735	-1.518125

11	8	0	-3.219943	-1.414744	0.000299
12	8	0	-4.185356	0.638572	-0.000245
13	6	0	-5.453251	-0.020653	-0.000417
14	1	0	-1.912880	1.641382	0.000076
15	1	0	-0.730874	-1.208716	0.000748
16	1	0	0.655610	2.326370	0.898829
17	1	0	0.654764	2.325865	-0.898619
18	1	0	4.647995	0.475638	-0.885498
19	1	0	4.727968	-1.066419	-0.000945
20	1	0	4.648827	0.476056	0.882962
21	1	0	3.055654	-1.878369	1.635646
22	1	0	1.273825	-1.721855	1.504387
23	1	0	2.211862	-0.502819	2.379851
24	1	0	3.054155	-1.879207	-1.635472
25	1	0	2.209676	-0.504065	-2.379647
26	1	0	1.272454	-1.722659	-1.502695
27	1	0	-5.568828	-0.650223	-0.888118
28	1	0	-6.200448	0.775288	-0.000668
29	1	0	-5.569184	-0.650001	0.887395

INT_{22g}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.950018	0.732418	-0.344206
2	6	0	0.934542	-0.086309	0.059648
3	7	0	-0.392184	0.143493	-0.004424
4	15	0	-2.042219	-0.861517	-0.029514
5	8	0	-2.340522	0.649384	-0.720948
6	6	0	-1.045965	1.270482	-0.624241
7	6	0	3.355884	0.387935	-0.217066
8	6	0	-3.848537	-1.289956	-0.284541
9	6	0	-1.317228	-2.258111	-0.986821
10	6	0	-1.961577	-1.173777	1.782945
11	8	0	4.285661	1.092667	-0.576014
12	8	0	3.562939	-0.842828	0.359493
13	6	0	4.935632	-1.214263	0.499116
14	6	0	-1.068619	2.530146	0.202038
15	6	0	-2.173878	3.130634	0.639502
16	1	0	1.763397	1.704606	-0.787393
17	1	0	1.200517	-1.044864	0.502253
18	1	0	-0.665586	1.478040	-1.638273
19	1	0	-4.487150	-0.593726	0.268331
20	1	0	-4.056412	-2.307425	0.064083
21	1	0	-4.115360	-1.219754	-1.343645
22	1	0	-1.949984	-3.147779	-0.918997
23	1	0	-0.305906	-2.491321	-0.648207
24	1	0	-1.260503	-1.950710	-2.036790
25	1	0	-2.663444	-1.955871	2.087145
26	1	0	-2.227994	-0.240595	2.290553
27	1	0	-0.944314	-1.436603	2.081669
28	1	0	5.430957	-1.263398	-0.475398
29	1	0	4.929193	-2.199154	0.970637
30	1	0	5.474957	-0.497383	1.125591
31	1	0	-0.085089	2.939931	0.426508
32	1	0	-3.160126	2.737641	0.411543
33	1	0	-2.124850	4.037693	1.235577

INT_{22h}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.797345	-0.448327	0.015534
2	6	0	3.136119	0.098318	-0.005068

3	8	0	3.483374	1.274597	-0.028803
4	6	0	0.644255	0.306708	0.042299
5	7	0	-0.581355	-0.274046	0.057537
6	6	0	-0.793957	-1.685957	-0.005949
7	8	0	-2.229894	-1.649606	-0.058403
8	15	0	-2.549052	-0.008123	-0.006154
9	6	0	-4.380675	-0.387188	-0.104248
10	6	0	-2.453892	1.076333	-1.489387
11	6	0	-2.582965	0.913126	1.585137
12	8	0	4.063868	-0.916414	0.003373
13	6	0	0.678463	1.819636	0.042642
14	6	0	5.424620	-0.486469	-0.018161
15	1	0	1.734941	-1.530777	0.019461
16	1	0	-0.396628	-2.171729	-0.909376
17	1	0	-0.466936	-2.244831	0.883014
18	1	0	-4.971651	0.534818	-0.079337
19	1	0	-4.610196	-0.924263	-1.029960
20	1	0	-4.685718	-1.021447	0.733860
21	1	0	-2.322984	0.422971	-2.359205
22	1	0	-1.600749	1.752644	-1.441332
23	1	0	-3.382778	1.640192	-1.618015
24	1	0	-3.507374	1.491368	1.677242
25	1	0	-1.714300	1.560659	1.699962
26	1	0	-2.560878	0.167668	2.387882
27	1	0	1.454207	2.186699	0.715107
28	1	0	-0.286483	2.246342	0.325600
29	1	0	0.945423	2.196531	-0.951480
30	1	0	6.023342	-1.399690	-0.018126
31	1	0	5.638039	0.106463	-0.913229
32	1	0	5.661337	0.120851	0.861364

INT₂₂i

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.656999	-0.094533	0.091037
2	6	0	3.078692	0.180878	-0.003907
3	8	0	3.659003	1.206927	-0.338148
4	6	0	0.630061	0.785319	-0.175923
5	7	0	-0.667728	0.391055	-0.065324
6	6	0	-1.847709	1.173746	-0.345856
7	8	0	-2.763346	0.052431	-0.337778
8	15	0	-1.731481	-1.243138	-0.047494
9	6	0	-2.251910	2.174979	0.699822
10	6	0	-3.215661	-2.391212	-0.114608
11	6	0	-1.165157	-1.719365	1.638338
12	6	0	-0.771331	-2.031021	-1.403393
13	6	0	-2.605581	3.430408	0.426300
14	8	0	3.786193	-0.942404	0.355228
15	6	0	0.872397	2.214547	-0.606625
16	6	0	5.206266	-0.800213	0.307743
17	1	0	1.423845	-1.099190	0.421827
18	1	0	-1.862435	1.636019	-1.343761
19	1	0	-2.240590	1.804377	1.724030
20	1	0	-2.908640	-3.432512	0.032175
21	1	0	-3.938306	-2.127367	0.664078
22	1	0	-3.721439	-2.308733	-1.081614
23	1	0	-1.826674	-1.217565	2.353849
24	1	0	-0.142376	-1.393932	1.830675
25	1	0	-1.260798	-2.799316	1.787408
26	1	0	-0.823018	-3.121061	-1.322999
27	1	0	0.267868	-1.699200	-1.417783
28	1	0	-1.248829	-1.736761	-2.345034
29	1	0	-2.894505	4.128833	1.206411
30	1	0	-2.617299	3.809283	-0.593766
31	1	0	1.939957	2.419377	-0.658704
32	1	0	0.396216	2.909693	0.093380

33	1	0	0.424220	2.393767	-1.592773
34	1	0	5.610024	-1.766803	0.615885
35	1	0	5.544892	-0.552920	-0.703273
36	1	0	5.547001	-0.013121	0.987682

INT_{22j}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.353397	-1.293527	0.138004
2	6	0	-2.676008	-0.374662	-0.675014
3	6	0	-3.424814	0.351938	-1.617402
4	6	0	-4.799381	0.162562	-1.745128
5	6	0	-5.460466	-0.757913	-0.928031
6	6	0	-4.733751	-1.483858	0.013257
7	15	0	-0.825355	-0.017021	-0.524105
8	6	0	-0.309722	-1.385196	0.581672
9	6	0	0.121862	-1.161675	1.895536
10	6	0	0.570406	-2.228907	2.676366
11	6	0	0.596768	-3.521530	2.152258
12	6	0	0.169778	-3.748186	0.841932
13	6	0	-0.283046	-2.687200	0.058612
14	6	0	-0.999615	1.586745	0.392233
15	6	0	-0.204855	2.704438	0.098278
16	6	0	-0.377581	3.902636	0.794327
17	6	0	-1.326528	3.994218	1.811245
18	6	0	-2.118919	2.885961	2.118829
19	6	0	-1.972555	1.699555	1.402945
20	8	0	-0.692881	-0.300561	-2.182522
21	6	0	0.710078	-0.075090	-2.394552
22	7	0	1.006101	0.363690	-1.065773
23	6	0	2.229147	0.371646	-0.495194
24	6	0	3.432371	0.182424	-1.106830
25	6	0	4.649951	0.253134	-0.314086
26	8	0	4.734933	0.473176	0.885883
27	1	0	0.551072	2.633074	-0.673545
28	1	0	-2.620788	0.860910	1.632630
29	1	0	-2.862351	2.947423	2.908877
30	1	0	-1.451674	4.923562	2.360417
31	1	0	0.240173	4.760475	0.543512
32	1	0	1.209652	-1.011035	-2.685521
33	1	0	0.852238	0.682294	-3.177440
34	1	0	2.235593	0.571171	0.574892
35	1	0	3.524608	-0.006423	-2.171036
36	8	0	5.754917	0.035169	-1.092562
37	1	0	0.109968	-0.159719	2.313672
38	1	0	0.904446	-2.044833	3.693640
39	1	0	0.950531	-4.349104	2.760816
40	1	0	0.188192	-4.752575	0.427707
41	1	0	-0.620518	-2.870882	-0.958048
42	1	0	-2.927218	1.066750	-2.266307
43	1	0	-5.355459	0.732764	-2.484923
44	1	0	-6.532535	-0.906821	-1.026705
45	1	0	-5.235647	-2.204738	0.653754
46	1	0	-2.810011	-1.874735	0.875945
47	6	0	7.001145	0.083919	-0.395121
48	1	0	7.768767	-0.111119	-1.146503
49	1	0	7.157668	1.066156	0.061544
50	1	0	7.039948	-0.673991	0.393399

INT_{22k}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-3.464521	-1.310098	-0.348414
2	6	0	-2.691721	-0.266470	-0.873640
3	6	0	-3.313816	0.641477	-1.749443
4	6	0	-4.658588	0.510166	-2.087461
5	6	0	-5.417287	-0.534659	-1.552760
6	6	0	-4.816749	-1.442346	-0.683532
7	15	0	-0.862628	-0.002030	-0.465707
8	6	0	-0.578665	-1.474111	0.593782
9	6	0	-0.714613	-1.439121	1.986876
10	6	0	-0.493678	-2.593837	2.741687
11	6	0	-0.139378	-3.787741	2.113389
12	6	0	-0.006206	-3.826908	0.723308
13	6	0	-0.224484	-2.677474	-0.034524
14	6	0	-1.088538	1.571276	0.481073
15	6	0	-0.214359	2.658230	0.335057
16	6	0	-0.437195	3.846331	1.033359
17	6	0	-1.518136	3.955727	1.907660
18	6	0	-2.392948	2.878859	2.064729
19	6	0	-2.194714	1.704478	1.340320
20	8	0	-0.537357	-0.110517	-2.105385
21	6	0	0.888088	0.071787	-2.145727
22	7	0	1.079211	0.279370	-0.745147
23	6	0	2.294627	0.250396	-0.131920
24	6	0	3.455398	0.170060	-0.868775
25	6	0	4.805051	0.159946	-0.337536
26	8	0	5.186386	0.203963	0.826339
27	1	0	0.642308	2.567819	-0.321503
28	1	0	-2.908732	0.893881	1.439352
29	1	0	-3.240924	2.956586	2.739546
30	1	0	-1.682300	4.876662	2.460637
31	1	0	0.243444	4.682215	0.897973
32	1	0	1.371547	-0.831640	-2.545667
33	1	0	1.132109	0.932199	-2.785387
34	6	0	2.278281	0.315578	1.375662
35	1	0	3.399300	0.130425	-1.951143
36	8	0	5.707841	0.090053	-1.372816
37	1	0	-0.980987	-0.514544	2.489580
38	1	0	-0.595576	-2.554716	3.822786
39	1	0	0.034421	-4.683600	2.702881
40	1	0	0.270560	-4.753009	0.227185
41	1	0	-0.121755	-2.717446	-1.115596
42	1	0	-2.738941	1.458202	-2.177034
43	1	0	-5.115585	1.222621	-2.769510
44	1	0	-6.467059	-0.638417	-1.814463
45	1	0	-5.395315	-2.261209	-0.263456
46	1	0	-3.020652	-2.034908	0.325606
47	6	0	7.078507	0.072408	-0.974962
48	1	0	7.653945	0.002609	-1.900390
49	1	0	7.344238	0.985181	-0.432181
50	1	0	7.291774	-0.785898	-0.330050
51	1	0	3.258926	0.600162	1.752855
52	1	0	1.517379	1.019138	1.725706
53	1	0	2.031720	-0.669178	1.789554

INT₂₂l

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.919731	0.103125	0.032651
2	15	0	1.037927	0.191827	0.076838
3	6	0	0.809802	0.639180	1.849522
4	7	0	-0.811692	-0.344460	-0.112685
5	6	0	-0.412637	-1.626851	-0.599828
6	8	0	1.004679	-1.386674	-0.516755
7	6	0	-2.064864	0.111924	0.055346
8	6	0	-3.238010	-0.538888	-0.193749
9	6	0	-4.491157	0.152551	0.057973

10	8	0	-5.562593	-0.640803	-0.251077
11	6	0	-6.840463	-0.037957	-0.034955
12	6	0	0.787956	1.698524	-0.954145
13	8	0	-4.627772	1.290787	0.486920
14	6	0	3.641802	0.502161	-1.102143
15	6	0	5.033428	0.398812	-1.146696
16	6	0	5.732976	-0.113965	-0.054246
17	6	0	5.030547	-0.529460	1.077452
18	6	0	3.639425	-0.423879	1.116046
19	1	0	1.632645	1.261859	2.209467
20	1	0	0.768066	-0.275859	2.449232
21	1	0	-0.142388	1.159386	1.971734
22	1	0	-0.701729	-1.838103	-1.639468
23	1	0	-0.692814	-2.474416	0.042063
24	1	0	-2.140557	1.130093	0.437839
25	1	0	-3.275026	-1.553464	-0.575595
26	1	0	-6.973139	0.234940	1.016514
27	1	0	-7.576152	-0.789781	-0.327042
28	1	0	-6.957176	0.864078	-0.643587
29	1	0	1.605898	2.410787	-0.821005
30	1	0	-0.164944	2.161859	-0.690325
31	1	0	0.735799	1.407855	-2.008234
32	1	0	3.122104	0.895190	-1.971807
33	1	0	5.569301	0.718239	-2.036792
34	1	0	6.816353	-0.192806	-0.085800
35	1	0	5.564203	-0.938412	1.931537
36	1	0	3.116755	-0.765757	2.005428

INT_{22m}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.089841	0.002840	0.003025
2	15	0	-1.229771	0.288111	0.078106
3	6	0	-1.090622	1.593753	-1.210739
4	7	0	0.732911	-0.096031	-0.001090
5	6	0	0.422244	-1.478223	-0.184062
6	8	0	-1.010459	-1.346848	-0.182972
7	6	0	2.001435	0.386796	0.034547
8	6	0	3.088562	-0.456578	-0.055398
9	6	0	4.481716	-0.058810	-0.027025
10	8	0	5.283090	-1.171829	-0.119996
11	6	0	6.685758	-0.907681	-0.100357
12	6	0	-1.108344	1.012293	1.763915
13	8	0	4.971096	1.062238	0.064417
14	6	0	2.156060	1.887477	0.139653
15	6	0	-3.813594	-0.368163	1.146817
16	6	0	-5.183989	-0.625706	1.084315
17	6	0	-5.860713	-0.525702	-0.131494
18	6	0	-5.155156	-0.175215	-1.282646
19	6	0	-3.785021	0.082642	-1.213480
20	1	0	-1.994870	2.206453	-1.247710
21	1	0	-0.943240	1.115317	-2.184233
22	1	0	-0.218037	2.213863	-1.007439
23	1	0	0.732696	-2.139387	0.638580
24	1	0	0.757175	-1.904342	-1.140989
25	1	0	2.927436	-1.525075	-0.145058
26	1	0	6.977833	-0.260920	-0.933737
27	1	0	7.170888	-1.881852	-0.189672
28	1	0	6.983177	-0.421069	0.833983
29	1	0	-2.004596	1.588354	2.007826
30	1	0	-0.220963	1.639986	1.837491
31	1	0	-1.002339	0.196423	2.485989
32	1	0	2.055694	2.347744	-0.852176
33	1	0	1.394218	2.329641	0.788649
34	1	0	3.148862	2.140735	0.508020
35	1	0	-3.310665	-0.468382	2.104639

36	1	0	-5.720964	-0.907339	1.986375
37	1	0	-6.927947	-0.723897	-0.182234
38	1	0	-5.669344	-0.103705	-2.237559
39	1	0	-3.259616	0.341167	-2.128724

INT_{22n}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.884966	-0.547224	-0.085023
2	15	0	-1.016378	-0.237699	-0.047139
3	6	0	-0.792022	-0.776778	1.700999
4	7	0	0.692965	0.726611	-0.067918
5	6	0	0.021123	1.926196	-0.500548
6	8	0	-1.306957	1.349810	-0.513057
7	6	0	2.031472	0.468893	-0.116458
8	6	0	2.502765	-0.770245	0.260257
9	6	0	3.843168	-1.331934	0.302828
10	8	0	4.859648	-0.518372	-0.130784
11	6	0	6.163428	-1.104362	-0.066862
12	6	0	-0.460753	-1.495569	-1.267546
13	8	0	4.074486	-2.467342	0.695356
14	6	0	2.905724	1.601452	-0.607441
15	6	0	0.059631	3.095251	0.444292
16	6	0	-3.476541	-1.689945	-0.644074
17	6	0	-4.856054	-1.904539	-0.568967
18	6	0	-5.677062	-0.980638	0.073838
19	6	0	-5.108275	0.163458	0.636590
20	6	0	-3.732821	0.375578	0.555487
21	6	0	0.316135	4.346909	0.064868
22	1	0	-1.367555	-1.688608	1.886103
23	1	0	-1.202205	0.012494	2.340827
24	1	0	0.259875	-0.918357	1.951113
25	1	0	0.270733	2.251799	-1.521240
26	1	0	1.786193	-1.501223	0.615444
27	1	0	6.420758	-1.376940	0.960759
28	1	0	6.847080	-0.339377	-0.440111
29	1	0	6.220119	-2.002394	-0.688757
30	1	0	-0.807947	-2.491855	-0.982130
31	1	0	0.626574	-1.507071	-1.343991
32	1	0	-0.896087	-1.241904	-2.239411
33	1	0	2.655906	1.845669	-1.648507
34	1	0	2.725913	2.504560	-0.014762
35	1	0	3.958139	1.338207	-0.556053
36	1	0	-0.141025	2.853088	1.487292
37	1	0	-2.876297	-2.432460	-1.158784
38	1	0	-5.284420	-2.797292	-1.017480
39	1	0	-6.749319	-1.147268	0.133588
40	1	0	-5.737299	0.896703	1.135024
41	1	0	-3.315682	1.283733	0.979621
42	1	0	0.520154	4.595683	-0.974745
43	1	0	0.334169	5.170237	0.773157

INT_{22o}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.652587	2.031518	0.873849
2	6	0	-0.819707	1.282431	0.025812
3	6	0	0.019348	1.958627	-0.869559
4	6	0	0.021344	3.353942	-0.920988
5	6	0	-0.793299	4.089009	-0.060053
6	6	0	-1.626271	3.424668	0.842931
7	15	0	-0.857285	-0.559063	0.136571

8	7	0	0.995098	-0.782631	-0.326774
9	6	0	2.228228	-0.446109	0.095927
10	6	0	3.423699	-0.877523	-0.398703
11	6	0	4.654390	-0.385001	0.198753
12	8	0	5.750488	-0.915028	-0.426347
13	6	0	7.008699	-0.485212	0.097784
14	6	0	-2.731979	-0.793295	0.081975
15	6	0	-3.380944	-1.749426	0.876412
16	6	0	-4.757362	-1.963683	0.768391
17	6	0	-5.510661	-1.229376	-0.146778
18	6	0	-4.877756	-0.284974	-0.956935
19	6	0	-3.503897	-0.073189	-0.843477
20	6	0	-0.547104	-1.055481	1.887304
21	8	0	-0.766259	-1.623131	-1.176177
22	6	0	0.655082	-1.698440	-1.370591
23	8	0	4.754917	0.397192	1.133907
24	1	0	0.680035	1.396286	-1.519623
25	1	0	-2.329239	1.528215	1.558129
26	1	0	-2.262383	3.990243	1.518231
27	1	0	-0.779714	5.175083	-0.090863
28	1	0	0.671108	3.863488	-1.626944
29	1	0	1.010334	-2.727332	-1.214737
30	1	0	0.920131	-1.364929	-2.384414
31	1	0	2.256013	0.264091	0.921503
32	1	0	3.496257	-1.574324	-1.226941
33	1	0	-3.030520	0.668101	-1.481330
34	1	0	-5.453795	0.288299	-1.678802
35	1	0	-6.581667	-1.393600	-0.230979
36	1	0	-5.237533	-2.707377	1.399225
37	1	0	-2.818961	-2.348888	1.586932
38	1	0	7.767471	-0.992848	-0.500828
39	1	0	7.120046	0.600079	0.011350
40	1	0	7.109704	-0.760338	1.152169
41	1	0	0.374316	-0.585054	2.234438
42	1	0	-1.377691	-0.777056	2.539643
43	1	0	-0.408831	-2.140951	1.929305

INT_{22p}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.913372	-0.771423	0.017438
2	15	0	1.055837	-0.541492	0.254547
3	6	0	1.061131	-0.930167	2.054284
4	7	0	-0.912738	-0.906509	0.147259
5	6	0	-0.671869	-1.640510	-1.053220
6	8	0	0.763325	-1.549704	-1.042642
7	6	0	-2.149314	-0.475666	0.517017
8	6	0	-3.269876	-0.822066	-0.205725
9	6	0	-4.638794	-0.444533	0.092326
10	8	0	-5.477789	-0.968897	-0.862256
11	6	0	-6.859680	-0.657043	-0.686712
12	6	0	0.841243	2.206253	0.922243
13	8	0	-5.082457	0.231364	1.013925
14	6	0	-2.218223	0.355702	1.775736
15	6	0	0.901180	1.243587	-0.094710
16	6	0	0.859892	1.653880	-1.435270
17	6	0	0.745783	3.006846	-1.750552
18	6	0	3.811861	0.249704	0.364851
19	6	0	5.191840	0.053161	0.288179
20	6	0	5.702611	-1.174391	-0.134395
21	6	0	4.823220	-2.200757	-0.480278
22	6	0	3.443453	-2.001824	-0.404914
23	6	0	0.681348	3.962929	-0.734409
24	6	0	0.732923	3.561124	0.600453
25	1	0	1.976064	-0.561168	2.525302
26	1	0	1.052021	-2.022727	2.136681

27	1	0	0.171200	-0.543602	2.549919
28	1	0	-1.064573	-1.172153	-1.968449
29	1	0	-0.974102	-2.696737	-1.022874
30	1	0	-3.163162	-1.441258	-1.089416
31	1	0	-7.231344	-1.033606	0.271445
32	1	0	-7.379957	-1.146185	-1.512795
33	1	0	-7.027764	0.424096	-0.720566
34	1	0	0.881440	1.909788	1.966754
35	1	0	-2.013718	-0.271491	2.653388
36	1	0	-1.474713	1.158133	1.753562
37	1	0	-3.213888	0.779945	1.892943
38	1	0	0.921640	0.915569	-2.229942
39	1	0	0.709500	3.314599	-2.791863
40	1	0	3.439131	1.218381	0.686151
41	1	0	5.866277	0.863079	0.554267
42	1	0	6.776653	-1.328684	-0.196201
43	1	0	5.209674	-3.160206	-0.814714
44	1	0	2.774053	-2.805240	-0.692114
45	1	0	0.592948	5.016811	-0.982711
46	1	0	0.686993	4.299673	1.395959

INT_{42a}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	1.378261	-0.047906	0.098147
2	7	0	0.384055	1.385030	-0.059809
3	6	0	-0.892380	1.316877	-0.063676
4	6	0	-1.790104	0.109206	0.041016
5	6	0	-0.995431	-1.182775	0.249347
6	8	0	0.168852	-1.154457	-0.541542
7	1	0	2.431021	0.801227	0.611507
8	1	0	1.415338	-0.840690	1.286069
9	1	0	2.152551	-0.429720	-1.019655
10	1	0	-1.417628	2.272578	-0.200935
11	1	0	-2.528976	0.274092	0.838076
12	1	0	-2.363799	0.072061	-0.897810
13	1	0	-1.591863	-2.061409	-0.021787
14	1	0	-0.742275	-1.288951	1.323213

INT_{42b}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.120864	1.369502	-0.334500
2	6	0	-1.033479	0.185394	-0.606201
3	6	0	-0.353804	-1.150783	-0.286607
4	8	0	0.996153	-1.097588	-0.682910
5	15	0	1.968200	-0.110083	0.394983
6	7	0	1.092194	1.374609	0.056905
7	1	0	2.812577	0.661599	1.278386
8	1	0	1.620194	-0.993075	1.460753
9	1	0	3.048172	-0.434534	-0.454273
10	1	0	-0.566156	2.352963	-0.542850
11	6	0	-2.381359	0.373434	0.074749
12	1	0	-1.246581	0.258045	-1.689455
13	1	0	-0.852570	-1.974351	-0.807204
14	1	0	-0.453970	-1.354859	0.794867
15	8	0	-2.910890	-0.465515	0.766429

16	1	0	-2.875089	1.352744	-0.116100
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INT_{42c}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.565381	1.428273	-0.103667
2	7	0	0.289924	1.417283	-0.104749
3	15	0	-0.727820	-0.033054	0.027731
4	8	0	0.653063	-1.040046	0.643114
5	6	0	1.810529	-1.057179	-0.149215
6	6	0	2.535463	0.280084	-0.031226
7	6	0	-2.170766	1.055604	-0.592161
8	6	0	-1.064049	-1.299464	-1.307355
9	6	0	-1.496658	-0.307706	1.686553
10	1	0	2.030120	2.425839	-0.125776
11	1	0	2.455903	-1.883851	0.177788
12	1	0	1.582215	-1.243015	-1.215979
13	1	0	3.313470	0.408051	-0.797668
14	1	0	3.047583	0.363840	0.940002
15	1	0	-1.942825	1.477870	-1.577500
16	1	0	-3.103171	0.481435	-0.670951
17	1	0	-2.334651	1.896060	0.090158
18	1	0	-2.077154	-1.674062	-1.124236
19	1	0	-1.072126	-0.817626	-2.290177
20	1	0	-0.370065	-2.138573	-1.301129
21	1	0	-2.578750	-0.421208	1.580377
22	1	0	-1.058215	-1.169189	2.187506
23	1	0	-1.308401	0.591955	2.282370

INT_{42d}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.890416	0.244808	-0.655010
2	6	0	1.045430	-0.989875	-0.909215
3	7	0	-0.191302	-1.192023	-0.679013
4	15	0	-1.316413	-0.049127	0.086184
5	6	0	2.834196	-0.079512	0.504953
6	6	0	-2.721322	-1.212187	-0.461344
7	6	0	-2.114322	1.407173	-0.764514
8	6	0	-1.642621	-0.303847	1.888760
9	8	0	3.934092	-0.564164	0.364098
10	1	0	2.520429	0.412125	-1.538597
11	1	0	1.605170	-1.836647	-1.329418
12	1	0	2.418685	0.154047	1.506453
13	1	0	-3.703023	-0.819046	-0.166726
14	1	0	-2.592703	-2.201945	-0.011088
15	1	0	-2.714831	-1.346594	-1.548692
16	1	0	-1.526459	2.322225	-0.716813
17	1	0	-3.068220	1.572148	-0.251215
18	1	0	-2.346532	1.152820	-1.803164
19	1	0	-1.243939	0.517036	2.482394
20	1	0	-1.141304	-1.233445	2.179645
21	1	0	-2.714750	-0.430661	2.057765
22	6	0	0.981339	1.430792	-0.320291
23	8	0	0.051206	1.036254	0.647178

24	1	0	1.565347	2.278745	0.065891
25	1	0	0.506344	1.779410	-1.256337

INT_{42e}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.820129	-0.169969	0.264544
2	6	0	-0.839579	-0.344685	1.405837
3	7	0	0.434927	-0.362525	1.395990
4	15	0	1.492859	-0.207329	-0.010386
5	6	0	-2.187201	-1.547440	-0.290922
6	6	0	2.936528	-0.681905	1.120315
7	6	0	2.152796	1.472307	-0.422943
8	6	0	1.809407	-1.594405	-1.204820
9	8	0	-3.174941	-2.164274	0.036021
10	6	0	-1.183132	0.693705	-0.842633
11	8	0	0.064274	0.146858	-1.182075
12	6	0	-1.124003	2.177999	-0.527523
13	6	0	-1.585760	2.819331	0.546936
14	1	0	-2.746419	0.252144	0.667018
15	1	0	-1.308032	-0.481572	2.389852
16	1	0	-1.462571	-1.947668	-1.028734
17	1	0	3.885346	-0.658099	0.568393
18	1	0	2.797773	-1.690301	1.527013
19	1	0	3.005913	0.007201	1.968247
20	1	0	1.511067	2.213728	0.061108
21	1	0	2.091082	1.629530	-1.500822
22	1	0	3.178911	1.596979	-0.069856
23	1	0	1.520725	-1.308422	-2.214939
24	1	0	1.188820	-2.443091	-0.896854
25	1	0	2.857093	-1.900564	-1.160858
26	1	0	-1.814573	0.607324	-1.746131
27	1	0	-0.640702	2.751065	-1.319322
28	1	0	-1.491969	3.897881	0.643073
29	1	0	-2.078052	2.311164	1.372357

INT_{42f}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.156003	0.136411	-1.093486
2	6	0	0.173436	-0.997370	-1.302890
3	7	0	-1.026281	-1.110292	-0.893133
4	15	0	-1.883102	0.016203	0.180946
5	6	0	2.287169	-0.359664	-0.199185
6	6	0	-3.464796	-0.974126	-0.199228
7	6	0	-2.690614	1.611558	-0.356797
8	6	0	-1.890751	-0.419161	1.979639
9	8	0	2.335639	-1.445258	0.336396
10	8	0	3.251911	0.577826	-0.085359
11	6	0	0.430054	1.352146	-0.495553
12	8	0	-0.352444	0.937017	0.581587
13	6	0	4.357841	0.222468	0.762663
14	1	0	1.605216	0.403230	-2.061755
15	1	0	0.562065	-1.842172	-1.886691
16	1	0	-4.336727	-0.545081	0.312013

17	1	0	-3.347731	-2.013711	0.124281
18	1	0	-3.667301	-0.989595	-1.275935
19	1	0	-2.010778	2.461491	-0.387404
20	1	0	-3.473196	1.814591	0.383209
21	1	0	-3.185305	1.479216	-1.323646
22	1	0	-1.394182	0.350930	2.568332
23	1	0	-1.329884	-1.354044	2.084396
24	1	0	-2.912801	-0.587958	2.326827
25	1	0	1.154881	2.103801	-0.159617
26	1	0	-0.166725	1.818359	-1.302609
27	1	0	5.025804	1.084055	0.747407
28	1	0	4.865455	-0.665862	0.377570
29	1	0	4.010809	0.021494	1.779391

INT_{42g}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.136974	0.535169	-0.613415
2	6	0	0.344591	-0.322551	-1.586027
3	7	0	-0.801129	-0.836071	-1.410432
4	15	0	-1.794581	-0.632719	0.032686
5	6	0	2.117560	-0.370639	0.114734
6	6	0	-2.292080	-2.461746	-0.163820
7	6	0	-3.445044	0.049931	-0.393990
8	6	0	-1.461438	-0.808848	1.856812
9	8	0	1.851798	-1.061144	1.078026
10	8	0	3.334657	-0.341890	-0.465736
11	6	0	0.178135	1.313935	0.384765
12	8	0	-1.170906	1.094668	0.115954
13	6	0	4.321915	-1.209473	0.122009
14	6	0	0.503159	2.789680	0.324679
15	6	0	-0.364197	3.747333	0.004363
16	1	0	1.726232	1.230913	-1.218698
17	1	0	0.825430	-0.486261	-2.559110
18	1	0	-3.083100	-2.732467	0.546357
19	1	0	-1.429066	-3.110576	0.029877
20	1	0	-2.641445	-2.668558	-1.179445
21	1	0	-3.504783	1.110342	-0.153037
22	1	0	-4.219452	-0.510825	0.136717
23	1	0	-3.593166	-0.092056	-1.469078
24	1	0	-1.627624	0.141431	2.367061
25	1	0	-0.416726	-1.105496	1.992883
26	1	0	-2.097777	-1.589111	2.280763
27	1	0	0.440086	0.959256	1.395638
28	1	0	5.228656	-1.055819	-0.463202
29	1	0	3.997532	-2.251726	0.065042
30	1	0	4.488455	-0.944202	1.169051
31	1	0	1.536189	3.040890	0.572525
32	1	0	-0.071482	4.793492	-0.018168
33	1	0	-1.393184	3.504246	-0.239053

INT_{42h}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.131663	0.724103	0.830930

2	6	0	0.090064	1.595438	0.141769
3	7	0	-1.092878	1.242446	-0.193743
4	15	0	-1.809501	-0.363045	-0.115630
5	6	0	2.053176	0.070477	-0.190124
6	6	0	-3.278700	0.302695	-1.111493
7	6	0	-2.835794	-0.805757	1.370071
8	6	0	-1.372238	-1.661617	-1.368951
9	8	0	1.894755	0.069924	-1.392689
10	6	0	0.397784	-0.351371	1.657633
11	8	0	-0.378222	-1.120658	0.804389
12	6	0	0.505498	3.020991	-0.129197
13	8	0	3.095743	-0.523973	0.426019
14	6	0	4.008361	-1.221479	-0.439127
15	1	0	1.754178	1.347134	1.487139
16	1	0	-4.038729	-0.480889	-1.237009
17	1	0	-2.957342	0.635077	-2.105182
18	1	0	-3.737504	1.158943	-0.606198
19	1	0	-2.358851	-0.431420	2.278890
20	1	0	-2.861852	-1.896928	1.443093
21	1	0	-3.853671	-0.415911	1.298944
22	1	0	-1.166281	-2.607776	-0.866584
23	1	0	-0.447785	-1.337143	-1.856144
24	1	0	-2.162741	-1.775481	-2.113447
25	1	0	-0.189419	0.168860	2.440617
26	1	0	1.126170	-0.991474	2.173567
27	1	0	-0.309923	3.570706	-0.602236
28	1	0	1.380433	3.024481	-0.792665
29	1	0	0.802908	3.525092	0.799673
30	1	0	4.774054	-1.635330	0.217541
31	1	0	3.489733	-2.019281	-0.976820
32	1	0	4.452187	-0.533320	-1.163339

INT₄₂i

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.147786	0.754413	0.290344
2	6	0	-0.070051	0.695596	1.362241
3	7	0	1.089654	0.177218	1.233244
4	15	0	1.743734	-0.700013	-0.135377
5	6	0	-1.979740	-0.519557	0.260647
6	6	0	2.989657	-1.493121	1.053234
7	6	0	2.998993	0.243278	-1.111662
8	6	0	1.167115	-2.329297	-0.817025
9	8	0	-1.718834	-1.558197	0.831041
10	6	0	-0.476722	0.988069	-1.091462
11	8	0	0.447845	-0.025860	-1.335912
12	6	0	0.123847	2.373832	-1.265372
13	6	0	-0.070472	3.474500	-0.538038
14	6	0	-0.410574	1.345218	2.681778
15	8	0	-3.083522	-0.343517	-0.495273
16	6	0	-3.931943	-1.496849	-0.630505
17	1	0	-1.841683	1.574640	0.506920
18	1	0	3.701696	-2.119593	0.499762
19	1	0	2.475526	-2.124859	1.787354
20	1	0	3.544838	-0.727799	1.604167
21	1	0	2.855043	1.306560	-0.898677
22	1	0	2.818274	0.088285	-2.176452
23	1	0	4.019780	-0.043096	-0.847213

24	1	0	0.971146	-2.242582	-1.885535
25	1	0	0.225168	-2.569988	-0.315642
26	1	0	1.897228	-3.115420	-0.610491
27	1	0	-1.270139	0.899344	-1.853427
28	1	0	0.776370	2.424019	-2.137445
29	1	0	0.410101	4.414204	-0.797704
30	1	0	-0.714314	3.500160	0.337804
31	1	0	0.430517	1.260921	3.372058
32	1	0	-1.290186	0.853457	3.118935
33	1	0	-0.668582	2.402916	2.543437
34	1	0	-4.760846	-1.176070	-1.261860
35	1	0	-3.386131	-2.319352	-1.099779
36	1	0	-4.295249	-1.821979	0.347821

INT_{42j}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.208172	-2.273449	0.411338
2	6	0	-1.483075	-1.587221	-0.574134
3	6	0	-1.609042	-1.995837	-1.910616
4	6	0	-2.467871	-3.040266	-2.253848
5	6	0	-3.178670	-3.721750	-1.264921
6	6	0	-3.034462	-3.344568	0.070369
7	15	0	-0.355692	-0.200707	-0.051331
8	6	0	-0.249348	1.451038	-0.933194
9	6	0	-0.111347	2.631607	-0.187969
10	6	0	0.002405	3.867585	-0.825312
11	6	0	-0.066214	3.947469	-2.216660
12	6	0	-0.218835	2.781079	-2.967633
13	6	0	-0.284011	1.539949	-2.333106
14	7	0	0.700600	-0.625067	1.296494
15	6	0	1.920038	-0.978313	1.209718
16	6	0	2.807214	-1.064036	-0.020694
17	6	0	4.194407	-0.500318	0.253777
18	8	0	4.698509	0.427886	-0.337843
19	8	0	0.789266	-0.866713	-1.269195
20	6	0	2.120042	-0.411491	-1.218977
21	6	0	-1.655929	0.518603	1.191723
22	6	0	-1.478385	0.646588	2.576920
23	6	0	-2.471908	1.210121	3.387754
24	6	0	-3.670335	1.650923	2.831542
25	6	0	-3.869369	1.527563	1.453357
26	6	0	-2.873679	0.973299	0.652269
27	1	0	2.405890	-1.293102	2.142337
28	1	0	2.624456	-0.681848	-2.154060
29	1	0	2.190176	0.681101	-1.122736
30	1	0	2.936665	-2.144001	-0.197719
31	8	0	4.807500	-1.180205	1.248587
32	1	0	-0.557066	0.294405	3.025745
33	1	0	-2.303452	1.297918	4.458810
34	1	0	-4.443129	2.085011	3.461106
35	1	0	-4.800297	1.865063	1.003880
36	1	0	-3.051590	0.894128	-0.418507
37	1	0	-0.099732	2.588351	0.896282
38	1	0	0.131158	4.768434	-0.231252
39	1	0	0.002255	4.911935	-2.712977
40	1	0	-0.272599	2.833098	-4.052020
41	1	0	-0.349191	0.637692	-2.928966

42	1	0	-1.022268	-1.511454	-2.679996
43	1	0	-2.569099	-3.329673	-3.296660
44	1	0	-3.837579	-4.543593	-1.533070
45	1	0	-3.574165	-3.874748	0.850553
46	1	0	-2.128344	-1.971593	1.449769
47	6	0	6.126252	-0.716960	1.592649
48	1	0	6.458035	-1.360890	2.407247
49	1	0	6.796841	-0.804758	0.734074
50	1	0	6.093779	0.327158	1.914166

INT₄₂k

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.218305	-2.344736	0.232509
2	6	0	-1.498923	-1.588772	-0.704976
3	6	0	-1.562207	-1.957445	-2.057664
4	6	0	-2.354972	-3.031294	-2.463391
5	6	0	-3.060731	-3.781200	-1.521553
6	6	0	-2.977836	-3.443408	-0.170572
7	15	0	-0.458521	-0.167308	-0.099866
8	6	0	-0.430725	1.519283	-0.917912
9	6	0	-0.320439	2.671686	-0.125998
10	6	0	-0.264154	3.936303	-0.712731
11	6	0	-0.364337	4.071258	-2.097949
12	6	0	-0.491276	2.932181	-2.894367
13	6	0	-0.498513	1.664098	-2.311457
14	7	0	0.589664	-0.582346	1.239194
15	6	0	1.835845	-0.863376	1.206846
16	6	0	2.743913	-0.866689	-0.026298
17	6	0	4.074613	-0.197112	0.265607
18	8	0	4.211950	0.982176	0.515221
19	8	0	0.743161	-0.715030	-1.327944
20	6	0	2.036536	-0.190390	-1.212334
21	6	0	-1.822352	0.436210	1.136459
22	6	0	-1.683066	0.522411	2.528975
23	6	0	-2.722824	1.002074	3.335538
24	6	0	-3.930733	1.399040	2.766861
25	6	0	-4.091877	1.317111	1.380674
26	6	0	-3.050145	0.846745	0.584482
27	6	0	2.495436	-1.294185	2.497509
28	1	0	2.584306	-0.388125	-2.142935
29	1	0	2.041675	0.897766	-1.051666
30	1	0	2.928869	-1.921485	-0.265806
31	8	0	5.102268	-1.072622	0.197945
32	1	0	-0.753351	0.204383	2.985705
33	1	0	-2.582943	1.059307	4.412803
34	1	0	-4.739591	1.767794	3.392800
35	1	0	-5.029226	1.621811	0.921160
36	1	0	-3.199466	0.798543	-0.492484
37	1	0	-0.283416	2.583469	0.955092
38	1	0	-0.154812	4.815708	-0.083706
39	1	0	-0.340922	5.057420	-2.554240
40	1	0	-0.570821	3.027247	-3.974320
41	1	0	-0.548791	0.786060	-2.944149
42	1	0	-0.975206	-1.419327	-2.790291
43	1	0	-2.408032	-3.289487	-3.517932
44	1	0	-3.667921	-4.625360	-1.838204
45	1	0	-3.514105	-4.026453	0.573454

46	1	0	-2.186329	-2.075237	1.282362
47	6	0	6.405230	-0.510865	0.437576
48	1	0	7.103926	-1.341435	0.335503
49	1	0	6.625275	0.271149	-0.293596
50	1	0	6.459064	-0.082524	1.442001
51	1	0	3.074887	-2.213993	2.349335
52	1	0	3.196610	-0.519904	2.834291
53	1	0	1.742489	-1.451035	3.271691

INT₄₂l

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.014358	0.133499	-1.192967
2	6	0	2.316501	-0.084328	0.002423
3	6	0	2.797921	-1.040460	0.907768
4	6	0	3.972493	-1.741913	0.635212
5	6	0	4.660618	-1.522035	-0.559399
6	6	0	4.172160	-0.591943	-1.477800
7	15	0	0.805658	0.897427	0.388071
8	6	0	0.508134	1.342218	2.182943
9	7	0	-0.236800	1.241774	-1.006847
10	6	0	-1.339141	0.663531	-1.277553
11	6	0	-2.046471	-0.448980	-0.535321
12	6	0	-3.535817	-0.177824	-0.447835
13	8	0	-4.074256	0.882363	-0.687395
14	8	0	-0.008638	-0.712071	0.682794
15	6	0	-1.394991	-0.677381	-0.843357
16	6	0	1.615327	2.597727	0.084914
17	8	0	-4.198433	-1.278669	-0.030717
18	6	0	-5.619263	-1.120016	0.129393
19	1	0	2.646548	0.856585	-1.913766
20	1	0	2.242855	-1.247277	1.816101
21	1	0	4.342446	-2.470507	1.351968
22	1	0	5.569732	-2.077031	-0.775816
23	1	0	4.694409	-0.424679	-2.416159
24	1	0	0.128571	0.512580	2.777595
25	1	0	1.461329	1.687023	2.594745
26	1	0	-0.187640	2.186468	2.234258
27	1	0	-1.838154	0.986059	-2.200177
28	1	0	-1.901324	-1.365776	-1.126507
29	1	0	-1.741992	-1.625187	1.272198
30	1	0	-1.726078	0.126429	1.527614
31	1	0	2.481916	2.743079	0.741122
32	1	0	0.887193	3.392014	0.290825
33	1	0	1.937698	2.720267	-0.951052
34	1	0	-5.983291	-2.087172	0.476610
35	1	0	-5.838173	-0.339313	0.862480
36	1	0	-6.083664	-0.852938	-0.823438

INT₄₂m

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.418940	-0.089404	-0.127015
2	15	0	-0.621450	-0.648344	0.306430
3	8	0	1.038606	-1.387063	0.670596

4	6	0	1.904076	-0.718866	1.524663
5	6	0	2.349899	0.590752	0.846624
6	6	0	3.125695	0.288049	-0.429746
7	8	0	4.312329	-0.282025	-0.138836
8	6	0	5.110814	-0.659928	-1.274195
9	6	0	1.119070	1.432352	0.532429
10	7	0	-0.074716	1.003455	0.367684
11	6	0	-1.220255	-1.406847	1.900486
12	6	0	-0.382695	-1.576683	-1.288877
13	8	0	2.748567	0.517702	-1.559416
14	1	0	3.016064	1.156500	1.512104
15	6	0	1.358922	2.919340	0.439825
16	1	0	-0.405932	-1.593922	2.599989
17	1	0	-1.682199	-2.366660	1.645202
18	1	0	-1.990227	-0.775744	2.349663
19	1	0	0.441602	-1.075872	-1.804214
20	1	0	-1.275641	-1.561883	-1.911289
21	1	0	-0.061931	-2.598171	-1.075533
22	1	0	2.777220	-1.349426	1.737079
23	1	0	1.445448	-0.457601	2.499073
24	1	0	6.014336	-1.106932	-0.858979
25	1	0	5.356977	0.217258	-1.878328
26	1	0	4.573362	-1.381387	-1.894651
27	1	0	0.429574	3.445219	0.215058
28	1	0	1.782914	3.303085	1.377030
29	1	0	2.090743	3.120187	-0.353120
30	6	0	-2.883123	1.233521	-0.091478
31	6	0	-4.221057	1.544189	-0.355685
32	6	0	-5.134884	0.535887	-0.658095
33	6	0	-4.698063	-0.789718	-0.694549
34	6	0	-3.360962	-1.090064	-0.433018
35	1	0	-2.182060	2.027017	0.138707
36	1	0	-4.546943	2.581689	-0.326732
37	1	0	-6.174477	0.777605	-0.864838
38	1	0	-5.397013	-1.589393	-0.928883
39	1	0	-3.054041	-2.134982	-0.474536

INT_{42n}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.296343	-0.126012	-0.140668
2	15	0	-0.630778	-0.792755	-0.811489
3	8	0	1.124752	-0.995249	-1.354945
4	6	0	2.302603	-0.790897	-0.635148
5	6	0	2.928756	-2.121658	-0.231899
6	6	0	3.835687	-2.353005	0.717832
7	7	0	-0.138046	-0.880550	0.878348
8	6	0	0.937529	-0.449011	1.403457
9	6	0	1.160948	-0.619411	2.885512
10	6	0	2.074905	0.153644	0.594345
11	6	0	1.793845	1.564551	0.120890
12	8	0	2.927869	2.294886	0.094471
13	6	0	2.789355	3.638757	-0.401712
14	6	0	-1.099339	-2.518082	-1.223731
15	6	0	-0.780335	0.154910	-2.423926
16	8	0	0.713926	2.002236	-0.223262
17	1	0	2.990954	0.189245	1.187860
18	1	0	-1.096594	-3.125897	-0.315382

19	1	0	-0.366527	-2.917055	-1.926062
20	1	0	-2.096049	-2.545261	-1.671469
21	1	0	-0.205872	-0.362120	-3.193019
22	1	0	-0.365830	1.157062	-2.298692
23	1	0	-1.833462	0.234836	-2.706608
24	1	0	3.018924	-0.281206	-1.303679
25	1	0	2.588659	-2.943603	-0.860462
26	1	0	4.236171	-3.350145	0.879926
27	1	0	4.230457	-1.573209	1.365673
28	1	0	0.282045	-1.072703	3.348037
29	1	0	1.358894	0.352238	3.357918
30	1	0	2.038609	-1.253072	3.066825
31	1	0	3.789748	4.069460	-0.357206
32	1	0	2.418302	3.630563	-1.429771
33	1	0	2.096151	4.207235	0.223513
34	6	0	-3.282519	-0.967661	0.397730
35	6	0	-4.491733	-0.457746	0.874528
36	6	0	-4.735090	0.915958	0.843070
37	6	0	-3.756689	1.770938	0.335022
38	6	0	-2.553532	1.254330	-0.150845
39	1	0	-3.112669	-2.039016	0.456509
40	1	0	-5.241312	-1.135471	1.276783
41	1	0	-5.674843	1.315656	1.215947
42	1	0	-3.928191	2.844792	0.315968
43	1	0	-1.800244	1.940224	-0.525562

INT₄₂₀

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.759523	-2.385197	-0.625110
2	6	0	1.947466	-1.178502	0.060653
3	6	0	3.249200	-0.770492	0.382816
4	6	0	4.344217	-1.558513	0.028030
5	6	0	4.150156	-2.755046	-0.664404
6	6	0	2.856727	-3.164768	-0.992050
7	15	0	0.507252	-0.167428	0.564579
8	6	0	0.706923	0.126507	2.420764
9	7	0	-0.482676	-0.018742	-0.924758
10	6	0	-1.679237	-0.406713	-1.090731
11	6	0	-2.568553	-1.128172	-0.087720
12	6	0	-3.910687	-0.425617	0.053486
13	8	0	-4.283585	0.187337	1.029992
14	8	0	-0.478359	-1.593640	1.035522
15	6	0	-1.838998	-1.290803	1.251349
16	6	0	1.101624	1.600213	0.099831
17	6	0	1.850959	1.844690	-1.064159
18	6	0	2.231953	3.136972	-1.421855
19	6	0	1.843495	4.227264	-0.638774
20	6	0	1.073574	4.009545	0.501909
21	6	0	0.712371	2.708543	0.866066
22	8	0	-4.643687	-0.559707	-1.073768
23	6	0	-5.918262	0.108805	-1.065636
24	1	0	0.753090	-2.717069	-0.851932
25	1	0	3.412129	0.168906	0.902405
26	1	0	5.348056	-1.234147	0.288768
27	1	0	5.003787	-3.366057	-0.945981
28	1	0	2.699084	-4.096695	-1.528442
29	1	0	-0.221374	0.489408	2.872903

30	1	0	1.495988	0.852164	2.626577
31	1	0	0.940660	-0.838695	2.870852
32	1	0	-2.120602	-0.271561	-2.086807
33	1	0	-2.767916	-2.108087	-0.546945
34	1	0	-2.287613	-2.101432	1.837460
35	1	0	-1.980408	-0.368344	1.835422
36	1	0	2.140793	1.012507	-1.698424
37	1	0	2.824581	3.295060	-2.319829
38	1	0	2.134095	5.236127	-0.920583
39	1	0	0.753144	4.849095	1.114083
40	1	0	0.109705	2.573522	1.760306
41	1	0	-6.357047	-0.088902	-2.043772
42	1	0	-6.553440	-0.290220	-0.270643
43	1	0	-5.786426	1.182802	-0.911568

INT₄₂p

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.012545	-0.844347	-1.081344
2	6	0	1.909573	-1.198586	-0.280818
3	6	0	2.026773	-2.361597	0.492671
4	6	0	3.193637	-3.134917	0.471653
5	6	0	4.273474	-2.762964	-0.325993
6	6	0	4.177930	-1.608360	-1.107487
7	15	0	0.314337	-0.117161	-0.436114
8	6	0	-0.003121	-0.695534	-2.179545
9	8	0	-1.172104	0.901510	-0.780952
10	6	0	-1.909930	1.397036	0.293144
11	6	0	-2.626089	0.213732	0.964331
12	6	0	-1.589298	-0.818752	1.392414
13	6	0	-2.011288	-1.728834	2.519852
14	7	0	-0.415528	-0.967479	0.906249
15	6	0	1.222352	1.451003	-0.012415
16	6	0	-3.626287	-0.422202	0.004785
17	8	0	-3.541777	-1.534899	-0.469616
18	8	0	-4.641184	0.427014	-0.255741
19	6	0	-5.623342	-0.054614	-1.189691
20	1	0	-3.184991	0.556348	1.845965
21	1	0	-0.877431	-1.351845	-2.118596
22	1	0	0.844528	-1.245642	-2.584581
23	1	0	-0.271644	0.151115	-2.812843
24	1	0	-2.642025	2.128410	-0.070926
25	1	0	-1.281516	1.903378	1.046863
26	1	0	-6.353920	0.749044	-1.284715
27	1	0	-6.097322	-0.964334	-0.811879
28	1	0	-5.158051	-0.269348	-2.154966
29	1	0	-1.214752	-2.433955	2.763065
30	1	0	-2.269864	-1.144685	3.412764
31	1	0	-2.910271	-2.282947	2.221725
32	1	0	1.196188	-2.659114	1.121433
33	1	0	3.253755	-4.031643	1.084580
34	1	0	5.180235	-3.362651	-0.341052
35	1	0	5.012525	-1.301972	-1.733946
36	1	0	2.968791	0.055431	-1.693559
37	6	0	1.064906	2.621031	-0.769695
38	6	0	1.768652	3.779044	-0.434802
39	6	0	2.601343	3.796112	0.685535
40	6	0	2.742097	2.643966	1.460916

41	6	0	2.073906	1.472893	1.101894
42	1	0	0.378683	2.624443	-1.608673
43	1	0	1.654717	4.672394	-1.043526
44	1	0	3.136758	4.703210	0.953845
45	1	0	3.382947	2.650662	2.338696
46	1	0	2.219829	0.569789	1.686334

TS_{22a}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.283221	1.487179	0.206552
2	7	0	-0.587699	0.542592	0.594801
3	6	0	-1.678459	0.310746	-0.239349
4	6	0	-2.548329	-0.700088	-0.073004
5	1	0	0.053081	2.156166	-0.631943
6	1	0	0.904272	1.943287	0.977309
7	1	0	-1.815790	1.001129	-1.082427
8	1	0	-3.379828	-0.835980	-0.755806
9	1	0	-2.466790	-1.383988	0.767407
10	8	0	1.616989	0.531400	-0.508144
11	15	0	1.193484	-0.873559	0.048202
12	1	0	0.094304	-1.596569	-0.445531
13	1	0	1.289273	-1.149620	1.422243
14	1	0	2.258597	-1.667415	-0.437926

11k

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.729813	0.069217	0.000001
2	7	0	0.575539	-0.473448	-0.000002
3	6	0	-0.541778	0.373853	0.000000
4	6	0	-1.783476	-0.121758	0.000000
5	1	0	1.893235	1.157622	0.000004
6	1	0	2.617132	-0.564118	-0.000001
7	1	0	-0.367296	1.456502	-0.000004
8	1	0	-2.650387	0.530882	0.000001
9	1	0	-1.948811	-1.194630	0.000004

11l

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.833542	2.759762	0.000000
2	7	0	-1.088496	1.507571	0.000000
3	6	0	0.000000	0.634727	0.000000
4	6	0	-0.164679	-0.701735	0.000000
5	1	0	0.184875	3.175256	0.000000
6	1	0	-1.660347	3.469478	0.000000
7	1	0	1.011169	1.062391	0.000000
8	6	0	0.991955	-1.604286	0.000000
9	1	0	-1.158321	-1.140414	0.000000
10	8	0	0.912032	-2.819121	0.000000
11	1	0	1.983436	-1.097542	0.000000

11m

Center	Atomic	Atomic	Coordinates (Angstroms)		
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Number	Number	Type	X	Y	Z
1	6	0	-1.691610	0.222271	-0.000122
2	7	0	-0.600507	-0.467718	-0.000276
3	6	0	0.593313	0.232747	-0.000235
4	6	0	1.792198	-0.389169	-0.000026
5	6	0	-2.993131	-0.417158	-0.000002
6	6	0	3.037426	0.379601	0.000028
7	8	0	4.152116	-0.113395	0.000238
8	6	0	-4.139508	0.281250	0.000277
9	1	0	-1.680427	1.324615	-0.000078
10	1	0	0.555724	1.330667	-0.000481
11	1	0	1.856726	-1.473404	0.000255
12	1	0	-2.991606	-1.504490	-0.000138
13	1	0	2.905012	1.485937	-0.000167
14	1	0	-5.108169	-0.208487	0.000386
15	1	0	-4.142770	1.369093	0.000414

11n

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.395839	-0.628845	0.336621
2	7	0	2.792990	0.257195	-0.345987
3	6	0	1.464160	0.576020	-0.106062
4	6	0	0.430300	-0.282122	-0.193623
5	6	0	-0.947212	0.209385	-0.014479
6	8	0	-1.273917	1.360994	0.206168
7	8	0	-1.836517	-0.810806	-0.115427
8	6	0	-3.210968	-0.439074	0.058564
9	1	0	2.937733	-1.147681	1.188645
10	1	0	4.422536	-0.890290	0.077937
11	1	0	1.268163	1.632444	0.069923
12	1	0	0.575576	-1.331966	-0.426308
13	1	0	-3.510654	0.294321	-0.695164
14	1	0	-3.372301	-0.009251	1.051191
15	1	0	-3.781222	-1.361621	-0.056367

11o

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.011966	-1.308183	0.344940
2	7	0	2.601668	-0.362523	-0.396930
3	6	0	1.379798	0.276054	-0.138481
4	6	0	0.228119	-0.437559	-0.167739
5	6	0	-1.128513	0.110258	-0.015806
6	8	0	-1.460242	1.269139	0.167790
7	6	0	1.514894	1.761042	0.053335
8	8	0	-2.037185	-0.899655	-0.100156
9	6	0	-3.406018	-0.500981	0.045021
10	1	0	3.947104	-1.811707	0.095579
11	1	0	2.473000	-1.651903	1.237673
12	1	0	0.279179	-1.504213	-0.359817
13	1	0	0.541979	2.231916	0.180499
14	1	0	2.143349	1.965444	0.929953
15	1	0	2.031501	2.190846	-0.812811
16	1	0	-3.686833	0.212000	-0.735301
17	1	0	-3.989596	-1.417929	-0.046980
18	1	0	-3.573419	-0.036446	1.021030

11p

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.379906	-0.172763	0.126790
2	7	0	1.688406	0.735148	-0.456316
3	6	0	0.341261	0.924396	-0.135997
4	6	0	-0.533276	-0.110215	-0.224779
5	6	0	3.766242	-0.431155	-0.241003
6	6	0	-1.984658	-0.038158	-0.004385
7	8	0	-2.660098	0.932508	0.293879
8	6	0	4.505132	-1.373506	0.360585
9	6	0	0.002253	2.352110	0.195604
10	8	0	-2.530524	-1.274641	-0.175689
11	6	0	-3.947280	-1.347276	0.023724
12	1	0	1.956117	-0.787249	0.935281
13	1	0	-0.160516	-1.084104	-0.524739
14	1	0	4.172548	0.185080	-1.039682
15	1	0	5.535497	-1.562954	0.076126
16	1	0	4.098479	-1.989522	1.159758
17	1	0	-1.064242	2.476162	0.373787
18	1	0	0.565837	2.669314	1.082569
19	1	0	0.324226	2.997909	-0.629721
20	1	0	-4.472616	-0.698577	-0.683056
21	1	0	-4.214116	-2.391398	-0.145593
22	1	0	-4.212560	-1.044223	1.040722

15a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	-0.383628	-0.000001	0.000001
2	8	0	1.110399	0.000002	-0.000008
3	1	0	-1.042951	1.214239	-0.328042
4	1	0	-1.042859	-0.323007	1.215590
5	1	0	-1.042963	-0.891225	-0.887503

15b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	0.000486	-0.000358	0.191953
2	8	0	0.001856	-0.001943	1.693218
3	6	0	-0.536515	1.585229	-0.559661
4	6	0	-1.105826	-1.255363	-0.561814
5	6	0	1.640244	-0.327843	-0.563515
6	1	0	-1.553983	1.814900	-0.228034
7	1	0	-0.516465	1.550024	-1.654366
8	1	0	0.123080	2.387958	-0.215546
9	1	0	-0.796836	-2.252809	-0.233842
10	1	0	-1.087558	-1.216848	-1.656412
11	1	0	-2.129863	-1.085023	-0.215172
12	1	0	2.009662	-1.296984	-0.214036
13	1	0	2.346719	0.442818	-0.239676
14	1	0	1.595680	-0.335270	-1.658020

15c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	-0.014107	-0.020872	0.915082
2	8	0	-0.060877	-0.123838	2.415246
3	6	0	-1.645633	-0.399189	0.168638

4	6	0	1.175400	-1.205901	0.182315
5	6	0	0.481013	1.621463	0.274089
6	6	0	-1.858431	-0.548086	-1.210016
7	6	0	-3.129962	-0.850954	-1.695531
8	6	0	-4.198024	-1.010928	-0.808374
9	6	0	-3.991777	-0.869716	-0.564482
10	6	0	-2.719688	-0.565940	1.053256
11	6	0	1.535618	-2.308223	0.970439
12	6	0	2.408000	-3.275197	0.469965
13	6	0	2.928620	-3.147975	-0.819321
14	6	0	2.581817	-2.047765	-1.606782
15	6	0	1.710762	-1.078469	-1.108139
16	6	0	1.820163	2.023344	0.412549
17	6	0	2.217369	3.303517	0.031003
18	6	0	1.281149	4.199831	-0.490694
19	6	0	-0.052401	3.812687	-0.625933
20	6	0	-0.452187	2.530825	-0.243613
21	1	0	-1.033426	-0.434821	-1.908048
22	1	0	-3.287412	-0.966068	-2.764683
23	1	0	-5.187866	-1.249298	-1.188805
24	1	0	-4.819815	-0.998496	1.256435
25	1	0	-2.539583	-0.462317	2.119094
26	1	0	1.136161	-2.386294	1.977291
27	1	0	2.684907	-4.125069	1.088073
28	1	0	3.609371	-3.900756	-1.208167
29	1	0	2.995276	-1.940360	-2.606134
30	1	0	1.466904	-0.213358	-1.719094
31	1	0	2.552763	1.332377	0.820501
32	1	0	3.256276	3.602458	0.141294
33	1	0	1.591186	5.197902	-0.788890
34	1	0	-0.784282	4.508157	-1.028012
35	1	0	-1.492675	2.239787	-0.349045

15d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.034981	-0.774164	-1.449551
2	15	0	1.465549	0.195738	-0.000053
3	6	0	2.035184	-0.773340	1.449909
4	8	0	1.915954	1.628515	-0.000487
5	6	0	-0.357773	0.033032	0.000053
6	1	0	1.684253	-0.283739	-2.362281
7	1	0	1.661001	-1.803116	-1.432082
8	1	0	3.129529	-0.790950	-1.463307
9	1	0	1.684750	-0.282300	2.362420
10	1	0	3.129733	-0.790299	1.463429
11	1	0	1.661018	-1.802234	1.433159
12	6	0	-1.109575	1.215308	-0.000020
13	6	0	-2.504582	1.162110	-0.000033
14	6	0	-3.157574	-0.071336	0.000013
15	6	0	-2.414879	-1.255000	0.000073
16	6	0	-1.021252	-1.203204	0.000104
17	1	0	-0.585929	2.166891	-0.000085
18	1	0	-3.080805	2.083523	-0.000084
19	1	0	-4.243626	-0.112841	-0.000005
20	1	0	-2.921532	-2.216503	0.000097
21	1	0	-0.456435	-2.133065	0.000137

15e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.025956	1.619743	2.080259
2	15	0	-0.013222	1.208446	0.293840

3	6	0	-1.470511	0.125913	0.040847
4	8	0	-0.042878	2.401736	-0.619492
5	6	0	1.479729	0.179377	0.036253
6	6	0	-2.395173	0.530468	-0.931197
7	6	0	-3.537792	-0.233177	-1.176344
8	6	0	-3.764677	-1.404708	-0.453016
9	6	0	2.207604	0.411472	-1.139355
10	6	0	3.354710	-0.332999	-1.416461
11	6	0	3.787171	-1.312117	-0.520550
12	6	0	3.072764	-1.543994	0.657005
13	6	0	1.925241	-0.801254	0.935368
14	6	0	-2.846134	-1.815131	0.516797
15	6	0	-1.703998	-1.054037	0.762576
16	1	0	0.864344	2.210078	2.316752
17	1	0	-0.048464	0.731440	2.719035
18	1	0	-0.914950	2.223358	2.286222
19	1	0	-2.204141	1.445320	-1.484162
20	1	0	-4.250101	0.087388	-1.931929
21	1	0	-4.654213	-1.999441	-0.643446
22	1	0	1.869477	1.187492	-1.819575
23	1	0	3.913153	-0.145170	-2.329597
24	1	0	4.681852	-1.890585	-0.735232
25	1	0	3.411747	-2.299460	1.360914
26	1	0	1.389032	-0.988100	1.862186
27	1	0	-3.019304	-2.728309	1.080072
28	1	0	-0.994955	-1.391943	1.514023

Computational Methods: Synchronicities³ were quantified using a previously described approach.^{4,5} According to this method, synchronicity (S_y) is defined as

$$S_y = 1 - (2n - 1)^{-1} \sum_{i=1}^n \frac{|\delta B_i - \delta B_{av}|}{\delta B_{av}} \quad (1)$$

where n is the number of bonds directly involved in the transformation and δB_i stands for the relative variation of a given bond index B_i at the transition structure (TS) relative to the reactants and products, according to the following expression:

$$\delta B_i = \frac{B_i^{TS} - B_i^R}{B_i^P - B_i^R} \quad (2)$$

In eq. 2, the superscripts TS , R and P refer to the transition structure, reactant(s) and product(s), respectively. The average value of δB_i , denoted as δB_{av} in eq. 1, therefore is

$$\delta B_{av} = n^{-1} \sum_{i=1}^n \delta B_i \quad (3)$$

In this work, Wiberg indices⁶ B_i were evaluated using the natural bond orbital (NBO) method.⁷

Donor-acceptor interactions have been computed using the NBO method. The energies associated with these two-electron interactions were computed by means of the second-order perturbation energy $\Delta E_{\phi\phi^*}^{(2)}$ according to the following equation

$$\Delta E_{\phi\phi^*}^{(2)} = -n_{\phi} \frac{\langle \phi^* | \hat{F} | \phi \rangle^2}{\epsilon_{\phi^*} - \epsilon_{\phi}} \quad (4)$$

where ϕ^* and ϕ are the non-Lewis and Lewis localized orbitals, \hat{F} is the Fock operator, n_{ϕ} is the occupation of the ϕ localized orbital and ϵ_{ϕ^*} and ϵ_{ϕ} are the respective energies.

Nucleus-independent chemical shifts (NICS) as defined by Schleyer⁸ were computed at the ring points of electron density⁹ using the gauge invariant atomic orbital¹⁰ (GIAO) approach at the GIAO-B3LYP/6-31G**/B3LYP/6-31G* level.

Energy densities at selected bond points of electron density¹¹ were computed according to the following expression:

$$H(r_b) = \frac{1}{4} \nabla^2 \rho(r_b) - G(r_b) \quad (5)$$

where $H(r_b)$ is the total energy density at the bond point r_b , $\rho(r_b)$ and $G(r_b)$ standing for the electron density and kinetic energy density at the same point, respectively. According to eq. 5, if a given interatomic interaction has a negative value of $H(r_b)$, this interaction is covalent in nature, and a positive value of $H(r_b)$ at the corresponding bond point indicates an ionic bond.

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