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Synthesis and *In Vitro* Anticancer Evaluation of Novel Chrysin and 7-aminochrysin Derivatives

Szabolcs Mayer[1], Péter Keglevich[1]*, Péter Ábrányi-Balogh[2]*, Áron Szigetvári[3], Miklós Dékány[3], Csaba Szántay Jr.[3] and László Hazai[1]

[1] Department of Organic Chemistry and Technology, Faculty of Chemical Technology and Biotechnology, Budapest University of Technology and Economics, H-1111 Budapest, Gellért tér 4., Hungary; mayer.szabolcs@mail.bme.hu (S. M.); hazai@mail.bme.hu (L.H)

[2] Medicinal Chemistry Research Group, Institute of Organic Chemistry, Research Centre for Natural Sciences, H-1117 Budapest, Magyar tudósok krt. 2., Hungary

[3] Spectroscopic Research Department, Gedeon Richter Plc., H-1475 Budapest 10, P. O. Box 27, Hungary; szigetvaria@richter.hu (Á. S.); m.dekany@richter.hu (M. D.) cs.szantay@richter.hu (C.S.J)

* Correspondence: pkeglevich@mail.bme.hu (P.K); abranyi-balogh.peter@ttk.hu (P.Á.-B.)

Supplementary materials:

S.1. Chemistry

S.1.1. 2-((5-Hydroxy-4-oxo-2-phenyl-4*H*-chromen-7-yl)oxy)-*N*-phenylacetamide (**7**)

Chrysin (**1**) (100 mg, 0.39 mmol), 2-chloro-*N*-phenylacetamide (**2**) (71 mg, 0.42 mmol) and anhydrous potassium carbonate (56 mg, 0.41 mmol) were dissolved in DMF (4 mL). The reaction mixture was stirred at room temperature for 46 h, then, it was poured into water (30 mL). After filtering off the precipitate, the filtrate was extracted with DCM (3 x 30 mL). The combined organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The filtered precipitation and the crude product obtained by extraction were purified separately with preparative TLC (DCM : MeOH = 60 : 1). Combining the pure products 135 mg (89 %) of compound **7** was isolated as a white solid. M.p.: 227-228 °C. TLC (DCM : MeOH = 60 : 1); R_f = 0.41. IR (KBr) 3421, 3401, 1693, 1661, 1532, 1170, 831 cm^{-1}. ^1H NMR (499,9 MHz; DMSO-d_6) δ (ppm) 4.88 (s; 2H; C(7)-OC<u>H</u>$_2$); 6.51 (d; J = 2.3 Hz; 1H; H-6); 6.90 (d; J = 2.3 Hz; 1H; H-8); 7.07 (s; 1H; H-3); 7.07–7.10 (m; 1H; H-4''); 7.31–7.36 (m; 2H; H-3'', H-5''); 7.57–7.61 (m; 2H; H-3', H-5'); 7.61–7.66 (m; 3H; H-4', H-2'', H-6''); 8.09–8.13 (m; 2H; H-2', H-6'); 10.16 (s; 1H; C(1'')-N<u>H</u>); 12.84 (s; 1H; C(5)-O<u>H</u>). ^{13}C NMR (125.7 MHz; DMSO-d_6) δ (ppm) 67.2 (C(7)-O<u>C</u>H$_2$); 93.6 (C-8); 98.6 (C-6); 105.2 (C-10); 105.3 (C-3); 119.5 (C-2'', C-6''); 123.7 (C-4''); 126.4 (C-2', C-6'); 128.7 (C-3'', C-5''); 129.1 (C-3', C-5'); 130.5 (C-1'); 132.1 (C-4'); 138.2 (C-1''); 157.1 (C-9); 161.1 (C-5); 163.5 (C-2); 163.8 (C-7); 165.5 (C(1'')-NH-<u>C</u>O); 182.0 (C-4). EI-HRMS: M=387.11020 (delta=0.2 ppm; $C_{23}H_{17}O_5N$).

S.1.2. 2-((5-Hydroxy-4-oxo-2-phenyl-4*H*-chromen-7-yl)oxy)-*N*-(*o*-tolyl)acetamide (**8**)

Chrysin (**1**) (100 mg, 0.39 mmol), 2-chloro-*N*-(*o*-tolyl)acetamide (**3**) (76 mg, 0.41 mmol) and anhydrous potassium carbonate (56 mg, 0.41 mmol) were dissolved in DMF (4 mL). The reaction mixture was stirred at room temperature for 28 h, then, it was poured into water (30 mL). After filtering off the precipitate, the filtrate was extracted with DCM (3 x 30 mL). The combined organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The filtered precipitation and the crude product obtained by extraction were purified separately with preparative TLC (DCM : MeOH = 40 : 1). Combining the pure products 155 mg (98 %) of compound **8** was isolated as a white solid. M.p.: 236-237 °C. TLC (DCM : MeOH = 40 : 1); R_f = 0.51. IR (KBr) 3422, 3059, 1690, 1661, 1358, 1171, 1044, 753 cm^{-1}. ^1H NMR (499.9 MHz; DMSO-d_6) δ (ppm) 2.22 (s; 3H; C(2'')-C<u>H</u>$_3$); 4.91 (s; 2H; C(7)-OC<u>H</u>$_2$); 6.53 (d; J = 2.1 Hz; 1H; H-6); 6.91 (d; J = 2.1 Hz; 1H; H-8); 7.08 (s; 1H; H-3); 7.10–7.15 (m; 1H; H-4''); 7.17–7.21 (m; 1H; H-5''); 7.22–7.26 (m; 1H; H-3''); 7.40–7.43 (m; 1H; H-6''); 7.58–7.62 (m; 2H; H-3', H-

5′); 7.62–7.66 (m; 1H; H-4′); 8.09–8.13 (m; 2H; H-2′, H-6′); 9.60 (br s; 1H; C(1′′)-NH); 12.83 (br s; 1H; C(5)-OH). ^{13}C NMR (125.7 MHz; DMSO-d_6) δ (ppm) 17.6 (C(2′′)-$\underline{C}H_3$); 67.2 (C(7)-O$\underline{C}H_2$); 93.6 (C-8); 98.7 (C-6); 105.2 (C-10); 105.4 (C-3); 125.2 (C-6′′); 125.6 (C-4′′); 126.0 (C-5′′); 126.4 (C-2′, C-6′); 129.1 (C-3′, C-5′); 130.3 (C-3′′); 130.5 (C-1′); 132.1 (C-4′, C-2′′); 135.3 (C-1′′); 157.1 (C-9); 161.1 (C-5); 163.5 (C-2); 163.7 (C-7); 165.7 (C(1′′)-NH-$\underline{C}$O); 182.0 (C-4). HRMS: M-H=400.11924 (delta=0.49 ppm; $C_{24}H_{18}O_5N$). HR-ESI-MS-MS (CID=35%; rel. int. %): 342(61); 293(19); 253(100).

S.1.3. 2-((5-Hydroxy-4-oxo-2-phenyl-4*H*-chromen-7-yl)oxy)-*N*-(2-methoxyphenyl)acetamide (**9**)

Chrysin (**1**) (50 mg, 0.20 mmol), 2-chloro-*N*-(2-methoxyphenyl)acetamide (**4**) (41 mg, 0.21 mmol) and anhydrous potassium carbonate (28 mg, 0.21 mmol) were dissolved in DMF (2 mL). The reaction mixture was stirred at room temperature for 29 h, then, it was poured into water (15 mL). After filtering off the precipitate, the filtrate was extracted with DCM (3 x 15 mL). The combined organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The filtered precipitation and the crude product obtained by extraction were purified separately with preparative TLC (DCM : MeOH = 40 : 1). Combining the pure products 66 mg (80 %) of compound **9** was isolated as a white solid. M.p.: 214-215 °C. TLC (DCM : MeOH = 40 : 1); R_f = 0.43. IR (KBr) 3403, 3075, 1660, 1450, 1338, 1171, 832, 498 cm^{-1}. ^{1}H NMR (799.7 MHz; $CDCl_3$) δ (ppm) 3.91 (s; 3H; C(2′′)-OC$\underline{H}_3$); 4.71 (s; 2H; C(7)-OC$\underline{H}_2$); 6.51 (d; *J* = 2.3 Hz; 1H; H-6); 6.60 (d; *J* = 2.3 Hz; 1H; H-8); 6.71 (s; 1H; H-3); 6.91 (dd; *J* = 8.2, 1.2 Hz; 1H; H-3′′); 6.99 (ddd; *J* = 8.0, 7.5, 1.2 Hz; 1H; H-5′′); 7.10 (ddd; *J* = 8.2, 7.5, 1.6 Hz; 1H; H-4′′); 7.53–7.56 (m; 2H; H-3′, H-5′); 7.56–7.59 (m; 1H; H-4′); 7.89–7.92 (m; 2H; H-2′, H-6′); 8.40 (dd; *J* = 8.0, 1.6 Hz; 1H; H-6′′); 8.87 (br s; C(1′′)-N$\underline{H}$); 12.79 (s; 1H; C(5)-O$\underline{H}$). ^{13}C NMR (201.1 MHz; $CDCl_3$) δ (ppm) 55.9 (C(2′′)-O$\underline{C}H_3$); 67.8 (C(7)-O$\underline{C}H_2$); 92.9 (C-8); 99.4 (C-6); 106.1 (C-3); 106.7 (C-10); 110.1 (C-3′′); 119.9 (C-6′′); 121.1 (C-5′′); 124.6 (C-4′′); 126.4 (C-2′, C-6′); 126.5 (C-1′′); 129.2 (C-3′, C-5′); 131.1 (C-1′); 132.1 (C-4′); 148.2 (C-2′′); 157.9 (C-9); 162.4 (C-5); 162.6 (C-7); 164.4 (C-2); 164.7 (C(1′′)-NH-$\underline{C}$O); 182.5 (C-4). HRMS: M+H=418.12807 (delta=-1.1ppm; $C_{24}H_{20}O_6N$). HR-ESI-MS-MS (CID=35%; rel. int. %): 400(11); 295(100); 267(57); 255(38); 237(5); 136(9).

S.1.4. *N*-(3,5-Dimethoxyphenyl)-2-((5-hydroxy-4-oxo-2-phenyl-4*H*-chromen-7-yl)oxy)acetamide (**10**)

Chrysin (**1**) (100 mg, 0.39 mmol), 2-chloro-*N*-(3,5-dimethoxyphenyl)acetamide (**5**) (95 mg, 0.41 mmol) and anhydrous potassium carbonate (56 mg, 0.41 mmol) were dissolved in DMF (4 mL). The reaction mixture was stirred at room temperature for 35 h, then, it was poured into water (30 mL). The precipitate was filtered off to afford 169 mg (96 %) of compound **10** as a white solid. M.p.: 237-238 °C. TLC (DCM : MeOH = 40 : 1); R_f = 0.39. IR (KBr) 3288, 1665, 1613, 1376, 1159, 825 cm^{-1}. ^{1}H NMR (499.9 MHz; DMSO-d_6) δ (ppm) 3.72 (s; 6H; C(3′′)-OC$\underline{H}_3$, C(5′′)-OC$\underline{H}_3$); 4.86 (s; 2H; C(7)-OC$\underline{H}_2$); 6.26 (t; *J* = 2.3 Hz; 1H; H-4′′); 6.50 (d; *J* = 2.3 Hz; 1H; H-6); 6.89 (d; *J* = 2.3 Hz; 1H; H-8); 6.91 (d; *J* = 2.3 Hz; 2H; H-2′′, H-6′′); 7.07 (s; 1H; H-3); 7.57–7.62 (m; 2H; H-3′, H-5′); 7.62–7.66 (m; 1H; H-4′); 8.09–8.12 (m; 2H; H-2′, H-6′); 10.10 (s; 1H; C(1′′)-N$\underline{H}$); 12.79 (br s; 1H; C(5)-O$\underline{H}$). ^{13}C NMR (125.7 MHz; DMSO-d_6) δ (ppm) 55.0 (C(3′′)-O$\underline{C}H_3$, C(5′′)-O$\underline{C}H_3$); 67.1 (C(7)-O$\underline{C}H_2$); 93.6 (C-8); 95.6 (C-4′′); 97.8 (C-2′′, C-6′′); 98.6 (C-6); 105.2 (C-10); 105.3 (C-3); 126.4 (C-2′, C-6′); 129.1 (C-3′, C-5′); 130.5 (C-1′); 132.1 (C-4′); 139.9 (C-1′′); 157.1 (C-9); 160.4 (C-3′′, C-5′′); 161.1 (C-5); 163.5 (C-2); 163.8 (C-7); 165.6 (C(1′′)-NH-$\underline{C}$O); 182.0 (C-4). HRMS: M+H=448.13910 (delta=0.05 ppm; $C_{25}H_{22}O_7N$). HR-ESI-MS-MS (CID=55%; rel. int. %): 430(6); 412(3); 295(100); 267(5); 255(3).

S.1.5. 2-((5-Hydroxy-4-oxo-2-phenyl-4*H*-chromen-7-yl)oxy)-*N*-(2-(trifluoromethyl)phenyl)-acetamide (**11**)

Chrysin (**1**) (50 mg, 0.20 mmol), 2-chloro-*N*-(2-(trifluoromethyl)phenyl)acetamide (**6**) (49 mg, 0.21 mmol) and anhydrous potassium carbonate (28 mg, 0.20 mmol) were dissolved in DMF (2 mL). The reaction mixture was stirred at room temperature for 24 h, then, it was poured into water (30 mL). After filtering off the precipitate, the filtrate was extracted with DCM (3 x 30 mL). The

combined organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The filtered precipitation and the crude product obtained by extraction were purified separately with preparative TLC (DCM : MeOH = 40 : 1). Combining the pure products 84 mg (94 %) of compound **11** was isolated as a white solid. M.p.: 263 °C (decomp.). TLC (DCM : MeOH = 40 : 1); R_f = 0.64. IR (KBr) 3425, 3076, 1707, 1663, 1170, 1117, 766, 758 cm^{-1}. ^1H NMR (399.8 MHz; DMSO-d_6) δ (ppm) 4.92 (s; 2H; C(7)-OC<u>H</u>$_2$); 6.47 (br d; *J* = 1.4 Hz; 1H; H-6); 6.84 (br d; *J* = 1.4 Hz; 1H; H-8); 7.07 (s; 1H; H-3); 7.46–7.52 (m; 1H; H-4''); 7.57–7.67 (m; 4H; H-3', H-5', H-6'', H-4'); 7.69–7.75 (m; 1H; H-5''); 7.75–7.80 (m; 1H; H-3''); 8.08–8.13 (m; 2H; H-2', H-6'); 9.9 (br; C(1'')-N<u>H</u>); 12.8 (br; C(5)-O<u>H</u>). ^{13}C NMR (101.5 MHz; DMSO-d_6) δ (ppm) 67.0 (C(7)-O<u>C</u>H$_2$); 93.3 (br; C-8); 98.7 (C-6); 105.4 (C-3, C-10); 123.5 (q; $^1J_{FC}$ = 273.6 Hz; C(2'')-<u>C</u>F$_3$); 124.5 (q; $^2J_{FC}$ = 29.3 Hz; C-2''); 126.2–126.4 (m; C-3'', C-2', C-6'); 126.9 (C-4''); 129.1 (C-3', C-5'); 129.5 (C-6''); 130.5 (C-1'); 132.1 (C-4'); 133.1 (C-5''); 134.6 (C-1''); 157.2 (C-9); 161.3 (C-5); 163.4 (C-7, C-2); 166.8 (C(1'')-NH-<u>C</u>O); 182.0 (C-4). ^{19}F NMR (376.2 MHz; DMSO-d_6) δ (ppm; ref.: $CFCl_3$) -59.3. HRMS: M+H=456.10417 (delta=-2.6ppm; $C_{24}H_{17}O_5NF_3$). HR-ESI-MS-MS (CID=35%; rel. int. %): 416(4); 396(100); 368(3); 358(5); 352(20); 295(3); 267(7); 255(15); 237(2).

S.1.6. 5-Hydroxy-2-phenyl-7-(phenylamino)-4*H*-chromen-4-one (**12**)

Chrysin (**1**) (100 mg, 0.39 mmol), 2-chloro-*N*-phenylacetamide (**2**) (71 mg, 0.42 mmol) and anhydrous potassium carbonate (112 mg, 0.79 mmol) were dissolved in DMF (4 mL). The reaction mixture was stirred at 85 °C for 49 h, then, it was poured into water (30 mL). After filtering off the precipitate, the filtrate was diluted with saturated NaCl solution (10 mL) and extracted with DCM (3 x 30 mL). The combined organic layer was washed with water (20 mL), dried over $MgSO_4$ and concentrated *in vacuo*. The filtered precipitation and the crude product obtained by extraction were purified separately with preparative TLC (DCM : MeOH = 60 : 1). Combining the pure products 37 mg (29 %) of compound **12** was isolated as a yellow solid. M.p.: 233-236 °C. TLC (DCM : MeOH = 60 : 1); R_f = 0.70. IR (KBr) 3307, 3202, 1654, 1619, 1406, 1171, 744, 504 cm^{-1}. ^1H NMR (499.9 MHz; DMSO-d_6) δ (ppm) 6.32 (d; *J* = 1.9 Hz; 1H; H-6); 6.66 (d; *J* = 1.9 Hz; 1H; H-8); 6.94 (s; 1H; H-3); 7.09–7.14 (m; 1H; H-4''); 7.25–7.29 (m; 2H; H-2'', H-6''); 7.38–7.43 (m; 2H; H-3'', H-5''); 7.54–7.62 (m; 3H; H-3', H-5', H-4'); 8.05–8.09 (m; 2H; H-2', H-6'); 9.10 (s; 1H; C(7)-N<u>H</u>); 12.80 (s; 1H; C(5)-O<u>H</u>). ^{13}C NMR (125.7 MHz; DMSO-d_6) δ (ppm) 90.9 (C-8); 97.0 (C-6); 103.2 (C-10); 105.1 (C-3); 121.0 (C-2'', C-6''); 123.2 (C-4''); 126.3 (C-2', C-6'); 129.0 (C-3', C-5'); 129.4 (C-3'', C-5''); 130.7 (C-1'); 131.8 (C-4'); 140.1 (C-1''); 151.3 (C-7); 157.6 (C-9); 160.9 (C-5); 162.7 (C-2); 181.0 (C-4). EI-HRMS: M=329.10387 (delta=-2.4 ppm; $C_{21}H_{15}O_3N$).

S.1.7. 5-Hydroxy-2-phenyl-7-(*o*-tolylamino)-4*H*-chromen-4-one (**13**)

Chrysin (**1**) (50 mg, 0.20 mmol), 2-chloro-*N*-(*o*-tolyl)acetamide (**3**) (38 mg, 0.21 mmol) and anhydrous potassium carbonate (56 mg, 0.41 mmol) were dissolved in DMF (2 mL). The reaction mixture was stirred at 80 °C for 61 h, then, it was evaporated under reduced pressure. Water (30 mL) was added to the residue and it was extracted with DCM (30 mL). Then, saturated NaCl solution (20 mL) was added to the aqueous phase and it was extracted with DCM (2 x 20 mL). The combined organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The crude product was purified with preparative TLC (DCM : MeOH = 40 : 1) to give 31 mg (46 %) of compound **13** as a yellow solid. M.p.: 220-221 °C. TLC (DCM : MeOH = 40 : 1); R_f = 0.69. IR (KBr) 3417, 3059, 1660, 1450, 1172, 1045, 766 cm^{-1}. ^1H NMR (499.9 MHz; DMSO-d_6) δ (ppm) 2.22 (s; 3H; C(2'')-C<u>H</u>$_3$); 6,10 (d; *J* = 2.0 Hz; 1H; H-6); 6.24 (d; *J* = 2.0 Hz; 1H; H-8); 6.89 (s; 1H; H-3); 7.16–7.21 (m; 1H; H-4''); 7.25–7.30 (m; 2H; H-5'', H-6''); 7.33–7.36 (m; 1H; H-3''); 7.52–7.56 (m; 2H; H-3', H-5'); 7.57–7.61 (m; 1H; H-4'); 8.01–8.04 (m; 2H; H-2', H-6'); 8.61 (s; 1H; C(7)-N<u>H</u>); 12.81 (s; 1H; C(5)-O<u>H</u>). ^{13}C NMR (125.7 MHz; DMSO-d_6) δ (ppm) 17.6 (C(2'')-<u>C</u>H$_3$); 90.1 (C-8); 96.0 (C-6); 102.5 (C-10); 105.0 (C-3); 125.5 (C-6''); 125.6 (C-4''); 126.2 (C-2', C-6'); 126.8 (C-5''); 129.0 (C-3', C-5'); 130.7 (C-1'); 131.1 (C-3''); 131.7 (C-4'); 133.4 (C-2''); 137.9 (C-1''); 153.2 (C-7); 157.6 (C-9); 161.0 (C-5); 162.5 (C-2); 180.9 (C-4). HRMS: M+H=344.12840 (delta=0.81ppm; $C_{22}H_{18}O_3N$).

HR-ESI-MS-MS (CID=65%; rel. int. %): 326(32); 311(3); 288(4); 270(2); 242(100); 225(13); 209(8); 172(7); 158(3); 129(5).

S.1.8. 5-Hydroxy-7-((2-methoxyphenyl)amino)-2-phenyl-4*H*-chromen-4-one (**14**)

Chrysin (**1**) (150 mg, 0.59 mmol), 2-chloro-*N*-(2-methoxyphenyl)acetamide (**4**) (126 mg, 0.63 mmol) and anhydrous potassium carbonate (168 mg, 1.2 mmol) were dissolved in DMF (10 mL). The reaction mixture was stirred at 105 °C for 31 h, then, it was evaporated under reduced pressure. Water (30 mL) was added to the residue and it was extracted with DCM (4x 40 mL). The combined organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The crude product was purified with preparative TLC (DCM : MeOH = 40 : 1) to give 71 mg (33 %) of compound **14** as a yellow solid. M.p.: 156-157 °C. TLC (DCM : MeOH = 40 : 1); R_f = 0.90. IR (KBr) 3348, 2963, 1668, 1586, 1512, 1257, 1227, 1024, 736 cm^{-1}. ^1H NMR (499.9 MHz; DMSO-d_6) δ (ppm) 3.82 (s; 3H; C(2'')-OC<u>H</u>$_3$); 6.23 (d; *J* = 2.0 Hz; 1H; H-6); 6.42 (d; *J* = 2.0 Hz; 1H; H-8); 6.89 (s; 1H; H-3); 7.00 (ddd; *J* = 7.8, 7.3, 1.3 Hz; 1H; H-5''); 7.14 (dd; *J* = 8.3, 1.3 Hz; 1H; H-3''); 7.20 (ddd; *J* = 8.3, 7.3, 1.5 Hz; 1H; H-4''); 7.33 (dd; *J* = 7.8, 1.5 Hz; 1H; H-6''); 7.53–7.57 (m; 2H; H-3', H-5'); 7.57–7.61 (m; 1H; H-4'); 8.01–8.05 (m; 2H; H-2', H-6'); 8.53 (s; 1H; C(7)-N<u>H</u>); 12.77 (s; 1H; C(5)-O<u>H</u>). ^{13}C NMR (125.7 MHz; DMSO-d_6) δ (ppm) 55.4 (C(2'')-O<u>C</u>H$_3$); 90.6 (C-8); 96.6 (C-6); 102.5 (C-10); 105.0 (C-3); 112.2 (C-3''); 120.6 (C-5''); 124.3 (C-6''); 125.6 (C-4''); 126.2 (C-2', C-6'); 128.1 (C-1''); 129.0 (C-3', C-5'); 130.8 (C-1'); 131.7 (C-4'); 152.6, 152.7 (C-9, C-2''); 157.5 (C-7); 160.8 (C-5); 162.5 (C-2); 180.9 (C-4). HRMS: M+H=360.12216 (delta=-2.4 ppm; $C_{22}H_{18}O_4N$). HR-ESI-MS-MS (CID=55%; rel. int. %): 345(100); 344(25); 330(2); 328(48); 327(2); 240(2).

S.1.9. 7-((3,5-Dimethoxyphenyl)amino)-5-hydroxy-2-phenyl-4*H*-chromen-4-one (**15**)

Chrysin (**1**) (50 mg, 0.20 mmol), 2-chloro-*N*-(3,5-dimethoxyphenyl)acetamide (**5**) (48 mg, 0.21 mmol) and anhydrous potassium carbonate (56 mg, 0.41 mmol) were dissolved in DMF (4 mL). The reaction mixture was stirred at 90 °C for 58 h, then, it was evaporated under reduced pressure. Water (20 mL) was added to the residue and it was extracted with DCM (4 x 20 mL). The combined organic layer was washed with water (20 mL), dried over $MgSO_4$ and concentrated *in vacuo*. The crude product was purified with preparative TLC (DCM : MeOH = 40 : 1) to give 22 mg (29 %) of compound **15** as a yellow solid. M.p.: 202-203 °C. TLC (DCM : MeOH = 40 : 1); R_f = 0.68. IR (KBr) 3276, 2998, 2832, 1660, 1615, 1450, 1208, 1154, 673 cm^{-1}. ^1H NMR (799.7 MHz; DMSO-d_6) δ (ppm) 3.76 (s; 6H; C(3'')-OC<u>H</u>$_3$, C(5'')-OC<u>H</u>$_3$); 6.27 (t; *J* = 2.2 Hz; 1H; H-4''); 6.34 (d; *J* = 1.9 Hz; 1H; H-6); 6.39 (d; *J* = 2.2 Hz; 2H; H-2'', H-6''); 6.70 (d; *J* = 1.9 Hz; 1H; H-8); 6.94 (s; 1H; H-3); 7.55–7.58 (m; 2H; H-3', H-5'); 7.59–7.62 (m; 1H; H-4'); 8.06–8.09 (m; 2H; H-2', H-6'); 9.07 (s; 1H; C(7)-N<u>H</u>); 12.80 (s; 1H; C(5)-O<u>H</u>). ^{13}C NMR (201.1 MHz; DMSO-d_6) δ (ppm) 55.1 (C(3'')-O<u>C</u>H$_3$, C(5'')-O<u>C</u>H$_3$); 91.6 (C-8); 95.0 (C-4''); 97.5 (C-6); 98.9 (C-2'', C-6''); 103.3 (C-10); 105.1 (C-3); 126.3 (C-2', C-6'); 129.0 (C-3', C-5'); 130.7 (C-1'); 131.8 (C-4'); 141.9 (C-1''); 150.9 (C-7); 157.5 (C-9); 160.8 (C-5); 161.0 (C-3'', C-5''); 162.8 (C-2); 181.0 (C-4). HRMS: M+H=390.13374 (delta=0.4ppm; $C_{23}H_{20}O_5N$). HR-ESI-MS-MS (CID=65%; rel. int. %): 374(100); 357(7); 343(2).

S.2.10. *N*-(5-Hydroxy-4-oxo-2-phenyl-4*H*-chromen-7-yl)-2-(2-(trifluoromethyl)phenoxy)-acetamide (**20**)

Chrysin (**1**) (100 mg, 0.39 mmol), 2-chloro-*N*-(2-(trifluoromethyl)phenyl)acetamide (**6**) (98 mg, 0.41 mmol) and anhydrous potassium carbonate (112 mg, 0.81 mmol) were dissolved in DMF (4 mL). The reaction mixture was stirred at 75 °C for 9 h, then, it was poured into water (30 mL). After filtering off the precipitate, the filtrate was diluted with saturated NaCl solution (30 mL) and extracted with DCM (4 x 30 mL). The combined organic layer was washed with water (30 mL), dried over $MgSO_4$ and concentrated *in vacuo*. The filtered precipitation and the crude product obtained by extraction were purified separately with preparative TLC (DCM : MeOH = 60 : 1). Combining the pure products 50 mg (28 %) of compound **20** was isolated as a white solid. M.p.: 210-212 °C. TLC

(DCM : MeOH = 60 : 1); R_f = 0.71. IR (KBr) 3398, 3057, 1662, 1524, 1323, 1132, 759, 674 cm^{-1}. ^1H NMR (499.9 MHz; DMSO-d_6) δ (ppm) 4.99 (s; 2H; C(1'')-OC<u>H</u>$_2$); 6.90 (d; J = 1.7 Hz; 1H; H-6); 7.08 (s; 1H; H-3); 7.14 (t; J = 7.5 Hz; 1H; H-4''); 7.21 (d; J = 8.5 Hz; 1H; H-6''); 7.56–7.67 (m; 6H; H-3', H-5', H-4', H-5'', H-3'', H-8); 8.09–8.13 (m; 2H; H-2', H-6'); 10.69 (s; 1H; C(7)-N<u>H</u>); 12.71 (s; 1H; C(5)-O<u>H</u>). ^{13}C NMR (125.7 MHz; DMSO-d_6) δ (ppm) 67.0 (C(1'')-O<u>C</u>H$_2$); 97.3 (C-8); 101.1 (C-6); 105.5 (C-3); 106.5 (C-10); 113.6 (C-6''); 117.0 (q; $^2J_{FC}$ = 30.2 Hz; C-2''); 120.8 (C-4''); 123.6 (q; $^1J_{FC}$ = 272.1 Hz; C(2'')-<u>C</u>F$_3$); 126.5 (C-2', C-6'); 126.8 (q; $^3J_{FC}$ = 4.9 Hz; C-3''); 129.1 (C-3', C-5'); 130.5 (C-1'); 132.2 (C-4'); 134.0 (C-5''); 144.8 (C-7); 155.7 (C-1''); 156.6 (C-9); 160.2 (C-5); 163.8 (C-2); 166.7 (C(7)-NH-<u>C</u>O); 182.0 (C-4). HRMS: M+H=456.10404 (delta=-2.8ppm; $C_{24}H_{17}O_5NF_3$). HR-ESI-MS-MS (CID=35%; rel. int. %): 436(82); 416(59); 396(22); 388(100); 358(69); 314(25); 294(59); 266(76).

Table S1. Energy values obtained for the computation of the 1→2 transformation and the related dimerization. The E, ZPE, U, H and G values were computed using the B3LYP/6-31 (d,p) method and are given in Hartree.

ID	E	ZPE	U	H	G
1-H$^+$	-686.329374	-686.178589	-686.16757	-686.166626	-686.215244
2	-899.880062	-899.733174	-899.723225	-899.722281	-899.771061
TS2	-1586.200932	-1585.902769	-1585.880373	-1585.879429	-1585.958358
7	-1586.256283	-1585.954988	-1585.932413	-1585.931469	-1586.011925
TS17a	-1125.349621	-1125.064369	-1125.045192	-1125.044248	-1125.112469
18a	-1125.35433	-1125.068375	-1125.048709	-1125.047765	-1125.118161
TS18a	-1201.789305	-1201.479757	-1201.457341	-1201.456397	-1201.532498
19a	-1201.797901	-1201.48845	-1201.465642	-1201.464698	-1201.54203
TS19a	-2590.113717	-2589.788308	-2589.759818	-2589.758874	-2589.851482
12	-2590.165232	-2589.837609	-2589.806734	-2589.80579	-2589.907816
3	-939.196944	-939.021998	-939.010525	-939.009581	-939.061674
TS4	-1625.52009	-1625.193985	-1625.170077	-1625.169133	-1625.251148
8	-1625.575712	-1625.24654	-1625.222444	-1625.2215	-1625.304732
TS17b	-1164.667656	-1164.354786	-1164.333898	-1164.332954	-1164.404827
18b	-1164.674747	-1164.361023	-1164.339799	-1164.338855	-1164.411551
TS18b	-1241.110539	-1240.772878	-1240.749141	-1240.748197	-1240.825996
19b	-1241.118663	-1240.781652	-1240.757325	-1240.756381	-1240.836324
TS19b	-2629.43213	-2629.079031	-2629.048855	-2629.047911	-2629.143327
13	-2629.485447	-2629.129779	-2629.097511	-2629.096567	-2629.200609
4	-1014.404738	-1014.224854	-1014.212336	-1014.211391	-1014.266518
TS4	-1700.727676	-1700.396788	-1700.371816	-1700.370872	-1700.45534
9	-1700.782981	-1700.449208	-1700.423959	-1700.423015	-1700.509838
TS17c	-1239.871867	-1239.554095	-1239.532245	-1239.531301	-1239.60573
18c	-1239.879217	-1239.560714	-1239.538414	-1239.53747	-1239.613382
TS18c	-1316.307867	-1315.967261	-1315.941811	-1315.940867	-1316.025548
19c	-1316.322218	-1315.9798	-1315.954459	-1315.953515	-1316.03614
TS19c	-2704.685705	-2704.324267	-2704.291312	-2704.290368	-2704.393983
14	-2704.636492	-2704.276809	-2704.245624	-2704.24468	-2704.342729
5	-1128.933309	-1128.721617	-1128.706345	-1128.705401	-1128.76654
TS5	-1815.254057	-1814.891005	-1814.863317	-1814.862373	-1814.953056
10	-1815.309407	-1814.943366	-1814.915457	-1814.914513	-1815.007363
TS17d	-1354.402003	-1354.051998	-1354.027451	-1354.026507	-1354.107248
18d	-1354.406686	-1354.055926	-1354.030949	-1354.030004	-1354.112475
TS18d	-1430.842	-1430.467912	-1430.44005	-1430.439106	-1430.527921
19d	-1430.84801	-1430.474038	-1430.445694	-1430.444749	-1430.534964
TS19d	-2819.166854	-2818.776692	-2818.742856	-2818.741912	-2818.846318
15	-2819.219063	-2818.826551	-2818.790391	-2818.789447	-2818.902673

6	-1236.912454	-1236.760834	-1236.747375	-1236.746431	-1236.803828
TS6	-1923.233964	-1922.930973	-1922.905091	-1922.904147	-1922.991113
11	-1923.289504	-1922.983649	-1922.957479	-1922.956535	-1923.046153
TS17e	-1462.383761	-1462.093956	-1462.071161	-1462.070217	-1462.1469
18e	-1462.386967	-1462.096214	-1462.073139	-1462.072195	-1462.14961
TS18e	-1538.823451	-1538.508691	-1538.483047	-1538.482103	-1538.564499
19e	-1538.830415	-1538.516366	-1538.489914	-1538.48897	-1538.574152
TS19e	-2927.14196	-2926.812256	-2926.780573	-2926.779628	-2926.880775
16	-2927.200824	-2926.869055	-2926.834593	-2926.833648	-2926.943602
23-24 TS	-1462.375226	-1462.086156	-1462.063323	-1462.062379	-1462.13876
24	-1462.381425	-1462.091145	-1462.068118	-1462.067173	-1462.144064
24-20-H$^+$ TS	-1462.380416	-1462.090589	-1462.068037	-1462.067093	-1462.142715
20-H$^+$	-1462.413081	-1462.121694	-1462.098254	-1462.09731	-1462.17723

Coordinates of the Computed Structures

1-H$^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.425475	-1.144505	-0.000236
2	6	0	-1.080869	-1.687854	0.000051
3	6	0	0.009834	-0.853513	0.000016
4	6	0	-0.088820	0.563282	-0.000124
5	6	0	-1.412986	1.117833	0.000029
6	6	0	-2.523516	0.303661	-0.000065
7	1	0	-0.946351	-2.764562	0.000209
8	6	0	1.080570	1.384647	-0.000409
9	1	0	-3.514193	0.749691	0.000021
10	6	0	2.348622	0.670031	-0.000205
11	6	0	2.389380	-0.682547	-0.000376
12	1	0	3.271015	1.238628	0.000075
13	6	0	3.623649	-1.525648	0.000313
14	1	0	4.517305	-0.900239	-0.000357
15	1	0	3.644034	-2.173625	0.883237
16	1	0	3.643872	-2.175385	-0.881324
17	8	0	1.034492	2.654911	0.000095
18	8	0	-1.541859	2.470139	0.000224
19	8	0	-3.448771	-1.887131	0.000096
20	8	0	1.264249	-1.446320	-0.000007
21	1	0	-0.602910	2.820365	0.000901

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.696133	-0.004752	0.790177
2	1	0	-3.311200	0.783515	1.218148
3	1	0	-2.667172	-0.868648	1.453702
4	6	0	-1.316435	0.567935	0.466841
5	8	0	-1.176091	1.760711	0.215414
6	7	0	-0.315732	-0.360419	0.482098
7	17	0	-3.523904	-0.545324	-0.741398
8	1	0	-0.587741	-1.307072	0.711492
9	6	0	1.058391	-0.192377	0.196187
10	6	0	1.868390	-1.337719	0.264594
11	6	0	1.630891	1.043323	-0.143017
12	6	0	3.231962	-1.250170	-0.001793
13	6	0	2.999828	1.112984	-0.407473
14	1	0	1.008185	1.924294	-0.195205
15	6	0	3.807625	-0.022872	-0.339993
16	1	0	3.843774	-2.145287	0.055481
17	1	0	3.434736	2.073143	-0.669254
18	1	0	4.870742	0.045596	-0.547716
19	1	0	1.426784	-2.295907	0.525978

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.835951	0.528634	1.129791
2	6	0	-1.312136	-0.297221	0.066892
3	6	0	-2.633759	-0.201447	-0.322799
4	6	0	-3.559070	0.681459	0.275660
5	6	0	-3.076484	1.511405	1.334913
6	6	0	-1.759414	1.430515	1.748294
7	1	0	-0.634386	-0.959980	-0.456978
8	6	0	-4.923822	0.739753	-0.178188
9	1	0	-1.409391	2.060420	2.559373
10	6	0	-5.254227	-0.155878	-1.270949
11	6	0	-4.321766	-0.979183	-1.808146
12	1	0	-6.265355	-0.159181	-1.659551
13	6	0	-4.540049	-1.939459	-2.931322
14	1	0	-5.573009	-1.896863	-3.278373
15	1	0	-3.872742	-1.705699	-3.767616
16	1	0	-4.314139	-2.961188	-2.608225
17	8	0	-5.778611	1.517737	0.335690
18	8	0	-3.932097	2.371048	1.933766
19	8	0	0.395115	0.500841	1.548906
20	8	0	-3.039547	-1.017698	-1.360271
21	6	0	1.429104	-1.318154	1.556059
22	1	0	0.497357	-1.833244	1.401156
23	1	0	1.683734	-0.979575	2.545171
24	1	0	-4.808008	2.237048	1.468726
25	6	0	2.168196	-0.854112	0.336246
26	8	0	1.806750	-1.175264	-0.794588
27	7	0	3.256232	-0.070699	0.613935
28	17	0	2.546626	-3.242111	1.842628
29	1	0	3.423749	0.122956	1.591558
30	6	0	4.164134	0.536393	-0.275882
31	6	0	5.183978	1.322346	0.288300
32	6	0	4.099024	0.391168	-1.671555
33	6	0	6.121379	1.951710	-0.525679
34	6	0	5.047233	1.029202	-2.473032
35	1	0	3.316201	-0.212030	-2.107235
36	6	0	6.060162	1.809934	-1.914439
37	1	0	6.901376	2.554692	-0.070397
38	1	0	4.986996	0.909823	-3.551069
39	1	0	6.790909	2.300739	-2.549544
40	1	0	5.238355	1.437162	1.367776

7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.577162	1.391273	-0.247225
2	6	0	-1.096109	0.571233	0.761247
3	6	0	-2.385481	0.075082	0.583270
4	6	0	-3.165081	0.361376	-0.546537
5	6	0	-2.602239	1.199023	-1.552990
6	6	0	-1.318279	1.706679	-1.397846
7	1	0	-0.544378	0.299171	1.650264
8	6	0	-4.502547	-0.190641	-0.674997
9	1	0	-0.886646	2.347417	-2.157397
10	6	0	-4.931459	-1.027579	0.423815
11	6	0	-4.121727	-1.262068	1.486364
12	1	0	-5.918606	-1.471553	0.390912
13	6	0	-4.449316	-2.102324	2.674904
14	1	0	-5.451137	-2.522448	2.583610
15	1	0	-3.726106	-2.918527	2.772844
16	1	0	-4.394153	-1.502615	3.589327
17	8	0	-5.225924	0.048750	-1.675836
18	8	0	-3.318239	1.496798	-2.649620
19	8	0	0.673469	1.939820	-0.208915
20	8	0	-2.873759	-0.729488	1.579428
21	6	0	1.472130	1.782404	0.968092

22	1	0	0.887780	1.940538	1.877822
23	1	0	2.243871	2.561530	0.902070
24	1	0	-4.193831	1.025933	-2.536497
25	6	0	2.175358	0.426437	1.072331
26	8	0	2.554720	0.017807	2.167658
27	7	0	2.371082	-0.194712	-0.125103
28	17	0	4.233152	4.206712	0.546924
29	1	0	1.996868	0.299020	-0.926537
30	6	0	3.011658	-1.421558	-0.401890
31	6	0	3.042623	-1.840959	-1.741820
32	6	0	3.606103	-2.219934	0.587902
33	6	0	3.657800	-3.040938	-2.088551
34	6	0	4.217375	-3.420819	0.223312
35	1	0	3.584209	-1.895202	1.618149
36	6	0	4.249348	-3.840524	-1.107358
37	1	0	3.673327	-3.349520	-3.129534
38	1	0	4.674868	-4.032135	0.995861
39	1	0	4.728732	-4.776158	-1.377544
40	1	0	2.583918	-1.223054	-2.509182

TS17a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.689428	-1.511595	-0.406320
2	6	0	-0.399299	-1.079735	-1.250975
3	6	0	-1.549970	-0.585232	-0.691680
4	6	0	-1.783965	-0.528844	0.706948
5	6	0	-0.742100	-1.048720	1.550134
6	6	0	0.416086	-1.559651	1.021296
7	1	0	-0.281621	-1.121235	-2.327207
8	6	0	-3.009287	-0.024957	1.231796
9	1	0	1.168703	-1.963123	1.691273
10	6	0	-3.973496	0.431867	0.239415
11	6	0	-3.706040	0.352854	-1.083799
12	1	0	-4.922590	0.832295	0.575514
13	6	0	-4.612527	0.776584	-2.193960
14	1	0	-5.547564	1.173408	-1.796412
15	1	0	-4.132660	1.546158	-2.808225
16	1	0	-4.837206	-0.071177	-2.850325
17	8	0	-3.264090	0.023413	2.477290
18	8	0	-0.949874	-1.053452	2.892243
19	8	0	1.380777	-2.622519	-0.959747
20	8	0	-2.530936	-0.142694	-1.562848
21	6	0	2.760247	-2.630992	-0.627757
22	1	0	3.302449	-3.155298	-1.420377
23	1	0	2.958593	-3.153381	0.320945
24	1	0	-1.860700	-0.652082	3.013700
25	6	0	3.228692	-1.181457	-0.503022
26	8	0	4.422748	-0.886642	-0.329806
27	7	0	2.150072	-0.396473	-0.611246
28	6	0	2.120526	0.965732	-0.292430
29	6	0	1.346272	1.836074	-1.081571
30	6	0	2.793697	1.492407	0.827778
31	6	0	1.246084	3.189658	-0.758797
32	6	0	2.699246	2.848452	1.136418
33	1	0	3.398486	0.831483	1.438085
34	6	0	1.923278	3.704863	0.349249
35	1	0	0.642435	3.845403	-1.380516
36	1	0	3.229885	3.238248	2.001131
37	1	0	1.850271	4.760149	0.595354
38	1	0	0.830777	1.435787	-1.947610

18a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.674195	-1.287932	-0.217510
2	6	0	-0.378711	-0.793864	-1.130505
3	6	0	-1.587674	-0.374902	-0.659614
4	6	0	-1.940251	-0.337629	0.721720
5	6	0	-0.927672	-0.792398	1.643342
6	6	0	0.294293	-1.224892	1.215510
7	1	0	-0.182805	-0.816813	-2.196848
8	6	0	-3.211936	0.112443	1.150192
9	1	0	1.027501	-1.558003	1.944895
10	6	0	-4.122854	0.529448	0.086357
11	6	0	-3.751788	0.476779	-1.211328
12	1	0	-5.111898	0.884250	0.352001
13	6	0	-4.588634	0.871112	-2.386042
14	1	0	-5.571143	1.215733	-2.060116
15	1	0	-4.102672	1.672463	-2.953608
16	1	0	-4.718990	0.023340	-3.067700
17	8	0	-3.567827	0.159963	2.376920
18	8	0	-1.234440	-0.774013	2.970773
19	8	0	1.023654	-2.682249	-0.627169
20	8	0	-2.521004	0.039124	-1.603620
21	6	0	2.420328	-2.880059	-0.670212
22	1	0	2.710182	-3.405790	-1.588908
23	1	0	2.794654	-3.467801	0.183523
24	1	0	-2.172734	-0.417523	3.010168
25	6	0	3.052052	-1.500096	-0.630911
26	8	0	4.254195	-1.257981	-0.737462
27	7	0	2.036337	-0.618285	-0.452357
28	6	0	2.255556	0.764510	-0.195649
29	6	0	1.656590	1.739708	-1.002481
30	6	0	3.077165	1.157952	0.869524
31	6	0	1.868805	3.093692	-0.736114
32	6	0	3.298310	2.511778	1.121093
33	1	0	3.540240	0.400037	1.491693
34	6	0	2.691222	3.484360	0.322446
35	1	0	1.396966	3.843275	-1.364678
36	1	0	3.938910	2.806499	1.947139
37	1	0	2.859669	4.538250	0.522941
38	1	0	1.027166	1.431268	-1.828445

TS18a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.519108	0.761887	0.326939
2	6	0	0.285497	0.287717	-0.760643
3	6	0	1.611460	-0.000270	-0.541795
4	6	0	2.218931	0.038675	0.737934
5	6	0	1.377089	0.394093	1.841560
6	6	0	0.044918	0.687587	1.649816
7	1	0	-0.125005	0.253454	-1.761934
8	6	0	3.598372	-0.302057	0.910836
9	1	0	-0.577468	0.931849	2.504351
10	6	0	4.308587	-0.663611	-0.305767
11	6	0	3.679103	-0.685740	-1.503766
12	1	0	5.358039	-0.925162	-0.242920
13	6	0	4.296386	-1.045568	-2.815959
14	1	0	5.350183	-1.296605	-2.689221
15	1	0	3.777679	-1.901669	-3.260648
16	1	0	4.211602	-0.210822	-3.519945
17	8	0	4.171337	-0.296613	2.042994
18	8	0	1.911758	0.405193	3.086936
19	8	0	-0.736972	2.607284	0.010528
20	8	0	2.363133	-0.368984	-1.642654
21	6	0	-2.059586	2.879927	0.309893
22	1	0	-2.549998	3.519420	-0.445440
23	1	0	-2.212023	3.379219	1.286624
24	1	0	2.870256	0.142270	2.960141
25	6	0	-2.836113	1.568591	0.337835
26	8	0	-4.057425	1.480837	0.435839
27	7	0	-1.965860	0.509490	0.215577
28	6	0	-2.433174	-0.834737	0.086663
29	6	0	-3.497321	-1.121180	-0.782436
30	6	0	-1.830118	-1.880385	0.799355
31	6	0	-3.954749	-2.430684	-0.921509
32	6	0	-2.287750	-3.189625	0.643879
33	1	0	-1.005975	-1.664256	1.468658
34	6	0	-3.353145	-3.472935	-0.211986
35	1	0	-4.779648	-2.636552	-1.597551
36	1	0	-1.808521	-3.989155	1.201537
37	1	0	-3.708957	-4.492265	-0.327347
38	1	0	-3.963877	-0.318686	-1.339707
39	8	0	-0.756543	2.982280	-2.674915
40	1	0	-0.661636	2.829690	-1.698613
41	1	0	-1.471605	2.382741	-2.921926

19a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.331055	0.580321	-0.309869
2	6	0	-0.322703	-0.507821	0.288556
3	6	0	-1.706922	-0.565761	0.222150
4	6	0	-2.477725	0.415368	-0.425226
5	6	0	-1.791445	1.499961	-1.038748
6	6	0	-0.402762	1.562228	-0.997378
7	1	0	0.228631	-1.281161	0.807249
8	6	0	-3.924279	0.303649	-0.468559
9	1	0	0.102696	2.375810	-1.502300
10	6	0	-4.472800	-0.854093	0.203433
11	6	0	-3.668289	-1.759370	0.815120
12	1	0	-5.546557	-0.994530	0.214754
13	6	0	-4.117553	-2.985101	1.538427
14	1	0	-5.204468	-3.067309	1.516572
15	1	0	-3.681414	-3.878017	1.078612
16	1	0	-3.781571	-2.954545	2.580096
17	8	0	-4.641099	1.159329	-1.050376
18	8	0	-2.489267	2.451488	-1.687038
19	8	0	1.002404	2.472553	1.763443
20	8	0	-2.315541	-1.637277	0.830664
21	6	0	1.824457	2.906098	0.778802
22	1	0	2.713162	3.499662	1.105874
23	1	0	1.329274	3.572813	0.028042
24	1	0	-3.449232	2.187337	-1.598376
25	6	0	2.504929	1.774627	-0.035446
26	8	0	3.691898	1.809796	-0.348648
27	7	0	1.748662	0.621419	-0.312614
28	6	0	2.458086	-0.605555	-0.557301

29	6	0	3.270973	-1.142496	0.448351
30	6	0	2.321699	-1.266705	-1.781338
31	6	0	3.955286	-2.335804	0.216418
32	6	0	3.000738	-2.466666	-2.001106
33	1	0	1.687979	-0.840419	-2.552951
34	6	0	3.822349	-3.001175	-1.005964
35	1	0	4.585658	-2.753578	0.996204
36	1	0	2.892709	-2.978715	-2.952738
37	1	0	4.353187	-3.932323	-1.180384
38	1	0	3.335384	-0.618261	1.398634
39	8	0	2.367688	0.806588	3.143027
40	1	0	1.808502	1.494583	2.600189
41	1	0	1.826192	0.008683	3.098306

TS19a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.746819	-0.032989	0.019252
2	6	0	1.894299	0.760356	-0.117899
3	6	0	3.137509	0.136567	-0.104069
4	6	0	3.292733	-1.248466	0.044248
5	6	0	2.116550	-2.033780	0.182000
6	6	0	0.862703	-1.429481	0.161619
7	1	0	1.841918	1.832761	-0.237921
8	6	0	4.618573	-1.846210	0.050825
9	1	0	-0.014068	-2.051585	0.273618
10	6	0	5.712054	-0.912942	-0.099419
11	6	0	5.486693	0.418332	-0.237629
12	1	0	6.727367	-1.289383	-0.101861
13	6	0	6.529219	1.473280	-0.399717
14	1	0	7.526315	1.032695	-0.390725
15	1	0	6.382238	2.008616	-1.343465
16	1	0	6.454132	2.206919	0.409567
17	8	0	4.784412	-3.085654	0.179285
18	8	0	2.213346	-3.366837	0.322549
19	8	0	-0.788875	1.370689	3.241233
20	8	0	4.234884	0.947668	-0.243613
21	6	0	-0.849360	0.100940	2.613961
22	1	0	-1.410484	-0.621507	3.224099
23	1	0	0.165790	-0.276355	2.490008
24	1	0	3.192041	-3.570488	0.301802
25	6	0	-1.618954	0.244044	1.283365
26	8	0	-2.574708	1.067509	1.282212
27	7	0	-0.573530	0.541454	-0.019901
28	6	0	-0.649772	1.922921	-0.474119
29	6	0	-0.433517	2.998456	0.394578
30	6	0	-0.928955	2.162571	-1.822519
31	6	0	-0.502493	4.304841	-0.089473
32	6	0	-0.995702	3.472878	-2.302212
33	1	0	-1.087146	1.328719	-2.499276
34	6	0	-0.784246	4.546748	-1.436953
35	1	0	-0.335188	5.135892	0.589130
36	1	0	-1.212124	3.649647	-3.351384
37	1	0	-0.836685	5.565490	-1.808673
38	1	0	-0.225721	2.802871	1.440645
39	1	0	-1.630295	1.791516	2.984041
40	6	0	-2.710776	-1.419778	-0.197527
41	8	0	-3.728273	-2.116588	-0.226619
42	8	0	-2.162149	-0.883888	-1.252375
43	8	0	-2.092219	-1.191758	0.989012
44	1	0	-1.326050	-0.193546	-0.831770
45	19	0	-4.077027	-2.035767	-2.996956
46	19	0	-4.808707	-0.426407	1.936331

12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.146896	0.430925	0.282761
2	6	0	-2.487581	0.869785	0.281197
3	6	0	-3.494413	-0.081029	0.203203
4	6	0	-3.247045	-1.463213	0.131561
5	6	0	-1.886431	-1.887441	0.150061
6	6	0	-0.863069	-0.956480	0.221987
7	1	0	-2.751267	1.913960	0.369537
8	6	0	-4.340224	-2.406642	0.053289
9	1	0	0.165582	-1.296719	0.221828
10	6	0	-5.663745	-1.818723	0.060508
11	6	0	-5.834138	-0.476065	0.140169
12	1	0	-6.527909	-2.469232	0.006243
13	6	0	-7.140680	0.245215	0.163704
14	1	0	-7.970193	-0.460135	0.107437
15	1	0	-7.233019	0.833022	1.082924
16	1	0	-7.205277	0.941394	-0.678980
17	8	0	-4.146851	-3.651027	-0.010850
18	8	0	-1.602603	-3.202991	0.087272
19	8	0	2.300445	1.014862	-3.880607
20	8	0	-4.785905	0.388063	0.209356
21	6	0	2.044988	-0.052124	-2.998310
22	1	0	2.410458	-0.990178	-3.431119
23	1	0	0.968558	-0.184487	-2.801681
24	1	0	-2.489587	-3.664859	0.035741
25	6	0	2.719826	0.181368	-1.657871
26	8	0	3.229133	1.245051	-1.362263
27	7	0	-0.069420	1.286888	0.381138
28	6	0	-0.030705	2.686224	0.262901
29	6	0	-0.858812	3.407657	-0.614613
30	6	0	0.936919	3.384152	1.008760
31	6	0	-0.737096	4.794086	-0.711843
32	6	0	1.060015	4.766452	0.890751
33	1	0	1.589291	2.830170	1.677423
34	6	0	0.217074	5.484333	0.038023
35	1	0	-1.386958	5.333845	-1.394640
36	1	0	1.814270	5.285028	1.475668
37	1	0	0.307645	6.562686	-0.045689
38	1	0	-1.575289	2.886385	-1.238334
39	1	0	2.568809	1.761684	-3.319445
40	6	0	3.117386	-0.758094	0.548598
41	8	0	4.074211	-1.495041	0.815578
42	8	0	2.430023	-0.000149	1.243011
43	8	0	2.672123	-0.900787	-0.865404
44	1	0	0.811129	0.849935	0.660908
45	19	0	3.976795	-0.599682	3.497060
46	19	0	4.414408	-3.317522	-1.181984

3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.650643	0.675492	0.380240
2	1	0	2.831968	0.827381	1.446178
3	1	0	2.521258	1.644589	-0.101057
4	6	0	1.432315	-0.241947	0.201703
5	8	0	1.524990	-1.462234	0.223959
6	7	0	0.268933	0.465325	0.076374
7	17	0	4.146849	-0.061560	-0.305886
8	1	0	0.365867	1.470084	0.048311
9	6	0	-1.065004	-0.008570	0.019774
10	6	0	-2.096175	0.959022	-0.036022
11	6	0	-1.373891	-1.376773	0.014273
12	6	0	-3.418194	0.508914	-0.096317
13	6	0	-2.705208	-1.788731	-0.044714
14	1	0	-0.571385	-2.098336	0.055717
15	6	0	-3.734015	-0.850585	-0.100908
16	1	0	-4.214644	1.246865	-0.139364
17	1	0	-2.930302	-2.851099	-0.048213
18	1	0	-4.770790	-1.168872	-0.148231
19	6	0	-1.796683	2.440565	-0.030137
20	1	0	-1.258621	2.750635	0.874672
21	1	0	-1.191565	2.744866	-0.893727
22	1	0	-2.723394	3.016689	-0.067871

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.005037	1.075396	0.478019
2	6	0	-1.531827	-0.220280	0.191709
3	6	0	-2.866023	-0.348013	-0.142294
4	6	0	-3.755480	0.745858	-0.223195
5	6	0	-3.221962	2.042105	0.056516
6	6	0	-1.891501	2.196186	0.400308
7	1	0	-0.882335	-1.087208	0.194916
8	6	0	-5.136448	0.549777	-0.579179
9	1	0	-1.502579	3.185004	0.619262
10	6	0	-5.521426	-0.824187	-0.842170
11	6	0	-4.621141	-1.833024	-0.754467
12	1	0	-6.547369	-1.038309	-1.115914
13	6	0	-4.895451	-3.279870	-1.005220
14	1	0	-5.941996	-3.432688	-1.271019
15	1	0	-4.263234	-3.652243	-1.818252
16	1	0	-4.663677	-3.871515	-0.113336
17	8	0	-5.959833	1.506471	-0.660760
18	8	0	-4.042136	3.115626	-0.009509
19	8	0	0.240558	1.276033	0.796104
20	8	0	-3.322409	-1.622422	-0.415294
21	6	0	1.209383	-0.140158	1.991677
22	1	0	0.255356	-0.590570	2.201687
23	1	0	1.499966	0.747250	2.526318
24	1	0	-4.936923	2.748107	-0.265860
25	6	0	1.940055	-0.611900	0.769396
26	8	0	1.545174	-1.580441	0.122446
27	7	0	3.055732	0.127605	0.476445
28	17	0	2.252220	-1.466937	3.471716
29	1	0	3.228748	0.905572	1.095370
30	6	0	3.972113	-0.020448	-0.586402
31	6	0	5.008398	0.938486	-0.697221
32	6	0	3.885558	-1.074444	-1.509695
33	6	0	5.927128	0.801226	-1.741582
34	6	0	4.820128	-1.179542	-2.539457
35	1	0	3.086185	-1.793521	-1.408973
36	6	0	5.846073	-0.244427	-2.662857
37	1	0	6.723287	1.535837	-1.829514

38	1	0	4.738682	-2.001023	-3.245347
39	1	0	6.574788	-0.323735	-3.463657
40	6	0	5.130204	2.087685	0.276133
41	1	0	4.252869	2.746090	0.248513
42	1	0	5.250556	1.743988	1.311469
43	1	0	6.002507	2.698954	0.036050

8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.644964	-1.365016	-0.277642
2	6	0	1.180812	-0.635511	0.789665
3	6	0	2.459543	-0.107594	0.626807
4	6	0	3.211807	-0.275415	-0.544555
5	6	0	2.630876	-1.020152	-1.611919
6	6	0	1.357260	-1.557977	-1.472808
7	1	0	0.649330	-0.456431	1.713822
8	6	0	4.540333	0.301999	-0.653344
9	1	0	0.913156	-2.131083	-2.277822
10	6	0	4.989916	1.035640	0.509195
11	6	0	4.205540	1.159273	1.608850
12	1	0	5.971431	1.492873	0.493818
13	6	0	4.554537	1.888752	2.862659
14	1	0	5.549670	2.327471	2.787377
15	1	0	3.825963	2.683481	3.053386
16	1	0	4.527711	1.205790	3.718023
17	8	0	5.239323	0.167357	-1.690468
18	8	0	3.320331	-1.202451	-2.749880
19	8	0	-0.596338	-1.935713	-0.258242
20	8	0	2.965620	0.605214	1.682076
21	6	0	-1.368247	-1.901799	0.946949
22	1	0	-0.755127	-2.116969	1.825618
23	1	0	-2.112304	-2.702787	0.836977
24	1	0	4.194384	-0.734601	-2.613707
25	6	0	-2.106748	-0.581142	1.182744
26	8	0	-2.497550	-0.298346	2.313201
27	7	0	-2.310507	0.152690	0.051479
28	17	0	-3.733514	-4.707453	0.470814
29	1	0	-1.918955	-0.260386	-0.784700
30	6	0	-2.966641	1.393991	-0.110905
31	6	0	-2.964298	1.971088	-1.402972
32	6	0	-3.603043	2.046059	0.955921
33	6	0	-3.609628	3.198815	-1.577265
34	6	0	-4.235922	3.271066	0.745182
35	1	0	-3.592715	1.586418	1.933612
36	6	0	-4.243644	3.854395	-0.520530
37	1	0	-3.610954	3.647126	-2.567196
38	1	0	-4.724595	3.764988	1.579916
39	1	0	-4.735809	4.807567	-0.687353
40	6	0	-2.287628	1.291890	-2.571053
41	1	0	-1.219024	1.122748	-2.388649
42	1	0	-2.738359	0.317697	-2.800016
43	1	0	-2.370337	1.905315	-3.470668

TS17b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.562986	-1.501804	-0.628126
2	6	0	-0.464606	-0.842750	-1.400524
3	6	0	-1.619275	-0.422436	-0.792787
4	6	0	-1.925865	-0.671353	0.571193
5	6	0	-0.956504	-1.427015	1.315485
6	6	0	0.208143	-1.863239	0.734512
7	1	0	-0.293385	-0.655774	-2.453458
8	6	0	-3.156286	-0.237038	1.143549
9	1	0	0.903208	-2.452470	1.324143
10	6	0	-4.045706	0.483387	0.241666
11	6	0	-3.711148	0.691572	-1.051980
12	1	0	-4.994464	0.846023	0.619063
13	6	0	-4.538153	1.402804	-2.073710
14	1	0	-5.479154	1.742049	-1.638671
15	1	0	-3.997012	2.269217	-2.469192
16	1	0	-4.755743	0.740797	-2.918872
17	8	0	-3.477028	-0.461521	2.354144
18	8	0	-1.239368	-1.730514	2.608412
19	8	0	1.247767	-2.484003	-1.391679
20	8	0	-2.533617	0.256641	-1.581179
21	6	0	2.608478	-2.626190	-1.014087
22	1	0	3.172558	-2.970970	-1.885989
23	1	0	2.744073	-3.364642	-0.208919
24	1	0	-2.137213	-1.317635	2.779708
25	6	0	3.111686	-1.267236	-0.527228
26	8	0	4.297993	-1.075867	-0.212222
27	7	0	2.070120	-0.429534	-0.510215
28	6	0	2.082795	0.810366	0.151764
29	6	0	1.891119	2.008359	-0.576056
30	6	0	2.232562	0.865705	1.548433
31	6	0	1.851767	3.217917	0.127900
32	6	0	2.189005	2.082007	2.229498
33	1	0	2.383182	-0.062020	2.090390
34	6	0	1.993733	3.265509	1.516955
35	1	0	1.711955	4.142313	-0.427594
36	1	0	2.305707	2.102984	3.309520
37	1	0	1.957652	4.219968	2.034385
38	6	0	1.759843	1.993687	-2.080214
39	1	0	2.571439	1.424205	-2.544571
40	1	0	0.824445	1.520579	-2.394071
41	1	0	1.778492	3.010717	-2.481641

18b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.504824	-1.245887	-0.499691
2	6	0	-0.345182	-0.260577	-1.201204
3	6	0	-1.607957	0.019610	-0.771476
4	6	0	-2.211934	-0.566002	0.380856
5	6	0	-1.399765	-1.510981	1.107254
6	6	0	-0.126955	-1.815205	0.718328
7	1	0	0.046634	0.211414	-2.095348
8	6	0	-3.528993	-0.233318	0.777704
9	1	0	0.448708	-2.534491	1.294575
10	6	0	-4.213403	0.742258	-0.067811
11	6	0	-3.606469	1.275441	-1.150258
12	1	0	-5.224848	1.037996	0.185513
13	6	0	-4.196520	2.278948	-2.088599
14	1	0	-5.211187	2.539946	-1.784215
15	1	0	-3.588086	3.189850	-2.110421
16	1	0	-4.223987	1.882291	-3.109537
17	8	0	-4.106243	-0.736416	1.801409
18	8	0	-1.948083	-2.091293	2.211125
19	8	0	0.871578	-2.333659	-1.457623
20	8	0	-2.336254	0.940175	-1.517031
21	6	0	2.222316	-2.710472	-1.290071
22	1	0	2.690383	-2.898236	-2.263700
23	1	0	2.344765	-3.618290	-0.676905
24	1	0	-2.869188	-1.694686	2.275487
25	6	0	2.900866	-1.540047	-0.595804
26	8	0	4.112517	-1.412550	-0.412678
27	7	0	1.908987	-0.696612	-0.222393
28	6	0	2.137181	0.537389	0.455189
29	6	0	2.784247	1.599392	-0.212318
30	6	0	1.708275	0.689493	1.779436
31	6	0	2.987387	2.791877	0.495212
32	6	0	1.909879	1.891608	2.456906
33	1	0	1.211055	-0.142407	2.264228
34	6	0	2.556321	2.946765	1.813140
35	1	0	3.487074	3.616749	-0.006149
36	1	0	1.571257	1.996648	3.483379
37	1	0	2.724113	3.886418	2.331412
38	6	0	3.252424	1.472017	-1.640260
39	1	0	4.096348	0.778364	-1.713319
40	1	0	2.460317	1.078691	-2.285534
41	1	0	3.566368	2.442124	-2.033534

TS18b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.337393	-0.901228	-0.165735
2	6	0	0.395210	-0.068673	0.746889
3	6	0	1.733319	0.158841	0.531284
4	6	0	2.430559	-0.298022	-0.614603
5	6	0	1.664738	-1.019285	-1.588432
6	6	0	0.322846	-1.258504	-1.398669
7	1	0	-0.090720	0.318240	1.633140
8	6	0	3.817921	-0.003856	-0.801069
9	1	0	-0.237062	-1.787731	-2.162892
10	6	0	4.441080	0.765985	0.264655
11	6	0	3.727818	1.181602	1.336989
12	1	0	5.492584	1.014966	0.186649
13	6	0	4.249761	1.982919	2.485141
14	1	0	5.308927	2.204906	2.349176
15	1	0	3.697763	2.924523	2.576429
16	1	0	4.118945	1.435324	3.424692
17	8	0	4.469796	-0.377685	-1.824026
18	8	0	2.285016	-1.433764	-2.720724
19	8	0	-0.617744	-2.519197	0.717837
20	8	0	2.404706	0.900204	1.487046
21	6	0	-1.880491	-2.927326	0.310314
22	1	0	-2.473923	-3.376126	1.124807
23	1	0	-1.868696	-3.668400	-0.511912
24	1	0	3.232909	-1.123540	-2.625644
25	6	0	-2.645073	-1.699041	-0.172421
26	8	0	-3.848077	-1.661846	-0.425020
27	7	0	-1.783351	-0.639110	-0.255455
28	6	0	-2.245978	0.686151	-0.537757
29	6	0	-3.098969	1.342836	0.374655
30	6	0	-1.825002	1.328138	-1.708574
31	6	0	-3.516261	2.642789	0.053722
32	6	0	-2.245691	2.624903	-1.997215
33	1	0	-1.160261	0.800187	-2.383669

34	6	0	-3.100854	3.284178	-1.112997
35	1	0	-4.173404	3.163096	0.745880
36	1	0	-1.911705	3.111823	-2.908563
37	1	0	-3.438589	4.294210	-1.326061
38	6	0	-3.563885	0.691865	1.653779
39	1	0	-4.385007	-0.004940	1.452212
40	1	0	-2.770038	0.108995	2.132416
41	1	0	-3.921261	1.446073	2.360145
42	8	0	-1.144269	-1.696405	3.251223
43	1	0	-0.884271	-2.002186	2.342264
44	1	0	-0.390089	-1.161734	3.528696

19b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.251884	-0.582083	-0.286630
2	6	0	0.408399	0.448424	0.398053
3	6	0	1.788472	0.541167	0.281389
4	6	0	2.543118	-0.348926	-0.501798
5	6	0	1.846996	-1.375493	-1.200409
6	6	0	0.463588	-1.470908	-1.105617
7	1	0	-0.136565	1.162178	1.002829
8	6	0	3.984461	-0.202741	-0.595479
9	1	0	-0.053723	-2.244193	-1.660473
10	6	0	4.543764	0.891256	0.168282
11	6	0	3.753657	1.711652	0.905406
12	1	0	5.614205	1.053815	0.144756
13	6	0	4.214497	2.868874	1.727572
14	1	0	5.296914	2.980724	1.660768
15	1	0	3.737112	3.792191	1.383299
16	1	0	3.933434	2.725046	2.775994
17	8	0	4.688631	-0.977052	-1.294792
18	8	0	2.531411	-2.240164	-1.974377
19	8	0	-0.666276	-2.778774	1.348268
20	8	0	2.405814	1.556848	0.970856
21	6	0	-1.749087	-3.008678	0.578673
22	1	0	-2.627720	-3.476485	1.090152
23	1	0	-1.561874	-3.707310	-0.280015
24	1	0	3.489582	-1.967245	-1.898657
25	6	0	-2.426204	-1.788353	-0.096661
26	8	0	-3.610596	-1.810764	-0.429712
27	7	0	-1.675892	-0.618070	-0.255742
28	6	0	-2.364146	0.603246	-0.589798
29	6	0	-3.288223	1.181870	0.303889
30	6	0	-2.074301	1.218355	-1.813941
31	6	0	-3.900223	2.382580	-0.086512
32	6	0	-2.691206	2.414132	-2.174126
33	1	0	-1.357308	0.748154	-2.479916
34	6	0	-3.612912	2.998855	-1.303985
35	1	0	-4.613112	2.844522	0.591763
36	1	0	-2.456937	2.879996	-3.126529
37	1	0	-4.102841	3.931282	-1.568677
38	6	0	-3.640947	0.549637	1.626152
39	1	0	-4.401617	-0.226533	1.482470
40	1	0	-2.783034	0.063205	2.103333
41	1	0	-4.048870	1.298313	2.311379
42	8	0	-1.094635	-1.183031	3.294825
43	1	0	-0.952858	-1.841730	2.508048
44	1	0	-0.565252	-0.423150	3.022367

TS19b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.637717	0.143051	-0.177650
2	6	0	1.835454	0.645472	0.341353
3	6	0	3.003837	-0.072244	0.106109
4	6	0	3.020875	-1.268039	-0.626703
5	6	0	1.791964	-1.749436	-1.150941
6	6	0	0.611722	-1.040968	-0.927241
7	1	0	1.874733	1.567550	0.905693
8	6	0	4.273566	-1.980115	-0.843209
9	1	0	-0.309983	-1.409906	-1.354924
10	6	0	5.437897	-1.367313	-0.247346
11	6	0	5.343324	-0.207999	0.452602
12	1	0	6.401764	-1.846441	-0.365238
13	6	0	6.470206	0.514206	1.110942
14	1	0	7.409574	-0.016365	0.954952
15	1	0	6.558369	1.527304	0.705375
16	1	0	6.283713	0.605252	2.185958
17	8	0	4.317829	-3.049211	-1.501214
18	8	0	1.763905	-2.882949	-1.869704
19	8	0	-1.438097	-0.615425	3.572673
20	8	0	4.161814	0.439331	0.631529
21	6	0	-0.576416	-0.262330	2.493435
22	1	0	-0.015510	-1.149729	2.201266
23	1	0	0.132948	0.519651	2.795194
24	1	0	2.709701	-3.207396	-1.901295
25	6	0	-1.471141	0.275936	1.361646
26	8	0	-2.412056	1.026889	1.685361
27	7	0	-0.618557	0.839085	0.071048
28	6	0	-0.499640	2.301267	0.013871
29	6	0	-0.429729	2.917989	-1.253348
30	6	0	-0.425351	3.070879	1.179681
31	6	0	-0.287601	4.312296	-1.295474
32	6	0	-0.288831	4.456725	1.107589
33	1	0	-0.497915	2.595619	2.148018
34	6	0	-0.220179	5.082331	-0.135693
35	1	0	-0.113180	6.160523	-0.204769
36	1	0	-2.088791	0.110760	3.590953
37	6	0	-2.813956	-1.030486	-0.329796
38	8	0	-3.767738	-1.815723	-0.438862
39	8	0	-2.514005	-0.112538	-1.208250
40	8	0	-1.995057	-1.123104	0.730517
41	1	0	-1.525845	0.448876	-0.731073
42	19	0	-4.676361	-0.809755	-2.842269
43	19	0	-3.483792	-2.540838	2.467835
44	1	0	-0.235670	5.037821	2.022856
45	1	0	-0.228744	4.797464	-2.265774
46	6	0	-0.484148	2.140363	-2.548344
47	1	0	-0.388609	2.819260	-3.398603
48	1	0	-1.426705	1.596312	-2.659971
49	1	0	0.322772	1.403433	-2.617009

13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.175336	0.221899	0.473671
2	6	0	-2.457245	0.791098	0.318710
3	6	0	-3.534800	-0.055134	0.108562
4	6	0	-3.415606	-1.455223	0.048272
5	6	0	-2.114140	-2.010719	0.221765
6	6	0	-1.019834	-1.185779	0.426756
7	1	0	-2.622017	1.857811	0.380891
8	6	0	-4.577532	-2.286595	-0.172840
9	1	0	-0.035264	-1.621629	0.551684
10	6	0	-5.829297	-1.572019	-0.316029
11	6	0	-5.877246	-0.219300	-0.239912
12	1	0	-6.739727	-2.134731	-0.481523
13	6	0	-7.101333	0.625973	-0.362481
14	1	0	-7.981727	0.005099	-0.530411
15	1	0	-7.248080	1.215350	0.548652
16	1	0	-6.995658	1.329507	-1.194862
17	8	0	-4.500120	-3.544008	-0.231167
18	8	0	-1.954625	-3.347845	0.175522
19	8	0	1.984569	2.381262	-2.902852
20	8	0	-4.766298	0.538277	-0.034732
21	6	0	1.902902	1.010366	-2.603023
22	1	0	2.344991	0.456326	-3.437187
23	1	0	0.867609	0.652707	-2.495138
24	1	0	-2.869935	-3.719964	0.012808
25	6	0	2.644433	0.647480	-1.322746
26	8	0	3.192300	1.446056	-0.595539
27	7	0	-0.049083	0.978724	0.718345
28	6	0	0.114275	2.372046	0.554356
29	6	0	0.910234	3.076791	1.486354
30	6	0	-0.438875	3.049347	-0.545952
31	6	0	1.115032	4.445803	1.282386
32	6	0	-0.228475	4.418955	-0.717613
33	1	0	-1.030548	2.498660	-1.269370
34	6	0	0.553860	5.123034	0.198512
35	1	0	0.725431	6.187449	0.072479
36	1	0	1.602428	2.866311	-2.154739
37	6	0	3.003563	-1.179121	0.231510
38	8	0	3.946091	-1.982254	0.178670
39	8	0	2.311995	-0.785679	1.182293
40	8	0	2.596564	-0.686683	-1.098465
41	1	0	0.786131	0.448596	0.972507
42	19	0	3.793054	-2.352147	2.965445
43	19	0	4.464783	-2.628755	-2.394723
44	1	0	-0.669486	4.925758	-1.570697
45	1	0	1.724543	4.991632	1.997836
46	6	0	1.529902	2.369617	2.666064
47	1	0	2.005882	3.085759	3.340243
48	1	0	2.290800	1.649294	2.344390
49	1	0	0.778595	1.808017	3.232534

4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.938480	0.238267	-0.770211
2	1	0	-3.640082	-0.301258	-1.402873
3	1	0	-2.702332	1.208456	-1.205906
4	6	0	-1.715515	-0.643788	-0.522269
5	8	0	-1.826619	-1.864908	-0.451410
6	7	0	-0.552121	0.051777	-0.388503
7	17	0	-3.800293	0.564669	0.803172
8	1	0	-0.593129	1.060491	-0.463136
9	6	0	0.743144	-0.440879	-0.127726
10	6	0	1.765576	0.535393	-0.026255

11	6	0	1.064215	-1.791508	0.030364
12	6	0	3.079438	0.148614	0.230292
13	6	0	2.385917	-2.169686	0.287302
14	1	0	0.277270	-2.527506	-0.049208
15	6	0	3.386837	-1.207902	0.386862
16	1	0	3.862884	0.892302	0.309415
17	1	0	2.622883	-3.221888	0.408281
18	1	0	4.413094	-1.500010	0.586166
19	8	0	1.345617	1.825386	-0.196851
20	6	0	2.306903	2.876607	-0.102489
21	1	0	1.754320	3.801534	-0.265776
22	1	0	2.772451	2.898267	0.888664
23	1	0	3.082276	2.773264	-0.869158

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.200656	1.033665	0.477276
2	6	0	-1.793621	-0.239746	0.220132
3	6	0	-3.131620	-0.306705	-0.115430
4	6	0	-3.963669	0.829222	-0.225600
5	6	0	-3.364126	2.102750	0.024166
6	6	0	-2.028328	2.196650	0.368671
7	1	0	-1.190628	-1.139065	0.247254
8	6	0	-5.351829	0.695817	-0.581772
9	1	0	-1.588879	3.169063	0.564724
10	6	0	-5.806044	-0.662669	-0.814227
11	6	0	-4.959068	-1.713887	-0.699258
12	1	0	-6.840601	-0.830644	-1.087801
13	6	0	-5.306115	-3.150092	-0.918837
14	1	0	-6.357834	-3.255087	-1.187474
15	1	0	-4.689704	-3.572412	-1.719504
16	1	0	-5.109445	-3.732711	-0.012671
17	8	0	-6.125408	1.691024	-0.688294
18	8	0	-4.127853	3.215145	-0.072003
19	8	0	0.051851	1.178023	0.794671
20	8	0	-3.652438	-1.562458	-0.358895
21	6	0	0.975106	-0.280705	1.983638
22	1	0	0.004175	-0.684071	2.211105
23	1	0	1.315733	0.596491	2.505404
24	1	0	-5.039750	2.887525	-0.321936
25	6	0	1.665038	-0.796728	0.756203
26	8	0	1.214921	-1.747431	0.116603
27	7	0	2.812260	-0.123310	0.445441
28	17	0	1.975863	-1.640350	3.465753
29	1	0	3.070772	0.654491	1.037817
30	6	0	3.693164	-0.336008	-0.629018
31	6	0	4.796559	0.551421	-0.712507
32	6	0	3.553067	-1.341970	-1.589962
33	6	0	5.727656	0.420085	-1.740326
34	6	0	4.493131	-1.465631	-2.618350
35	1	0	2.709389	-2.013110	-1.519444
36	6	0	5.573428	-0.592213	-2.695206
37	1	0	6.570513	1.097425	-1.804170
38	1	0	4.370393	-2.251538	-3.357043
39	1	0	6.303732	-0.686628	-3.492780
40	8	0	4.845692	1.500017	0.272796
41	6	0	5.923182	2.434852	0.266477
42	1	0	5.760744	3.084135	1.126593
43	1	0	6.888587	1.927223	0.368689
44	1	0	5.921668	3.034822	-0.650099

9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.790748	1.388369	0.360658
2	6	0	1.357472	0.794188	-0.772837
3	6	0	2.615488	0.213538	-0.630514
4	6	0	3.318196	0.199729	0.582986
5	6	0	2.707225	0.810765	1.716573
6	6	0	1.453980	1.398570	1.598875
7	1	0	0.864135	0.756387	-1.734001
8	6	0	4.626878	-0.424530	0.666644
9	1	0	0.986480	1.869259	2.455402
10	6	0	5.112464	-1.004812	-0.565985
11	6	0	4.376382	-0.954961	-1.704113
12	1	0	6.082397	-1.486367	-0.572481
13	6	0	4.766712	-1.513759	-3.031287
14	1	0	5.749268	-1.982823	-2.976597
15	1	0	4.032699	-2.256643	-3.360211
16	1	0	4.790317	-0.719235	-3.784272
17	8	0	5.281523	-0.452533	1.740525
18	8	0	3.349239	0.818410	2.896493
19	8	0	-0.433603	1.992588	0.367276
20	8	0	3.152991	-0.362832	-1.751812
21	6	0	-1.150413	2.137510	-0.863156
22	1	0	-0.495777	2.460843	-1.676470
23	1	0	-1.891942	2.926155	-0.676497
24	1	0	4.216866	0.347122	2.734450
25	6	0	-1.891102	0.874436	-1.309828
26	8	0	-2.210512	0.738451	-2.489984
27	7	0	-2.185761	0.013275	-0.298690
28	17	0	-3.679136	4.780653	-0.185241
29	1	0	-1.857376	0.274843	0.623734
30	6	0	-2.879952	-1.210908	-0.351641
31	6	0	-3.000273	-1.911622	0.874121
32	6	0	-3.440034	-1.754655	-1.510435
33	6	0	-3.671716	-3.131945	0.920274
34	6	0	-4.110890	-2.980750	-1.454854
35	1	0	-3.343300	-1.210485	-2.439095
36	6	0	-4.226918	-3.665491	-0.248909
37	1	0	-3.764870	-3.669225	1.856153
38	1	0	-4.541232	-3.392157	-2.362449
39	1	0	-4.747891	-4.616754	-0.203427
40	8	0	-2.418106	-1.294676	1.946977
41	6	0	-2.500111	-1.925214	3.224319
42	1	0	-1.980823	-1.263949	3.917637
43	1	0	-3.541917	-2.042876	3.541813
44	1	0	-2.008449	-2.904137	3.215069

TS17c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.160850	-0.793596	-0.702021
2	6	0	-0.563495	0.405861	-0.929281
3	6	0	-1.862654	0.478574	-0.472275
4	6	0	-2.473366	-0.541996	0.288626
5	6	0	-1.683708	-1.690378	0.597596
6	6	0	-0.371655	-1.786761	0.164146
7	1	0	-0.135742	1.221294	-1.499247
8	6	0	-3.826487	-0.402638	0.758594
9	1	0	0.199754	-2.669885	0.429022
10	6	0	-4.488766	0.833137	0.384281
11	6	0	-3.848019	1.778007	-0.344151
12	1	0	-5.510763	0.998589	0.702442
13	6	0	-4.415005	3.087437	-0.783064
14	1	0	-5.441718	3.198194	-0.432961
15	1	0	-3.812836	3.913499	-0.390324
16	1	0	-4.400188	3.161483	-1.875535
17	8	0	-4.396240	-1.292430	1.452178
18	8	0	-2.221171	-2.673296	1.343977
19	8	0	0.467558	-1.543626	-2.446470
20	8	0	-2.563620	1.624186	-0.770723
21	6	0	1.480687	-2.444955	-2.258523
22	1	0	2.175765	-2.518730	-3.117288
23	1	0	1.183399	-3.488056	-2.025242
24	1	0	-3.155387	-2.368927	1.548399
25	6	0	2.327471	-1.980951	-1.084922
26	8	0	3.271089	-2.418361	-0.507826
27	7	0	1.687004	-0.618476	-0.665300
28	1	0	1.869055	-0.006658	-1.475461
29	6	0	2.259753	0.037839	0.504563
30	6	0	2.813678	1.312770	0.285377
31	6	0	2.273134	-0.549395	1.763407
32	6	0	3.383382	2.000321	1.359237
33	6	0	2.841604	0.144316	2.833450
34	1	0	1.842281	-1.531632	1.911315
35	6	0	3.391175	1.408975	2.625027
36	1	0	3.813805	2.983487	1.216655
37	1	0	2.854720	-0.305690	3.819736
38	1	0	3.834782	1.950108	3.454646
39	8	0	2.734343	1.765818	-0.995559
40	6	0	3.304309	3.041051	-1.317207
41	1	0	3.133104	3.178891	-2.383677
42	1	0	2.809367	3.839951	-0.757108
43	1	0	4.378579	3.049376	-1.110050

18c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.079635	-0.745609	-0.147888
2	6	0	0.479953	0.457062	0.296413
3	6	0	1.856341	0.613084	0.194913
4	6	0	2.693627	-0.388284	-0.324791
5	6	0	2.097140	-1.597786	-0.772163
6	6	0	0.713487	-1.760782	-0.698147
7	1	0	-0.131966	1.240048	0.725243
8	6	0	4.131033	-0.173525	-0.406845
9	1	0	0.267005	-2.667906	-1.087114
10	6	0	4.591195	1.104329	0.086898
11	6	0	3.722438	2.022086	0.581856
12	1	0	5.650591	1.326880	0.058805
13	6	0	4.077814	3.367789	1.119010
14	1	0	5.153257	3.534930	1.057239
15	1	0	3.560207	4.149345	0.553367
16	1	0	3.761218	3.453565	2.163661
17	8	0	4.903792	-1.047269	-0.875120
18	8	0	2.860354	-2.573011	-1.290160
19	8	0	-0.474913	-2.224164	2.292273
20	8	0	2.383408	1.798690	0.640080
21	6	0	-1.386524	-2.890541	1.438885

22	1	0	-2.160549	-3.434104	1.993171
23	1	0	-0.809115	-3.627437	0.872831
24	1	0	3.799261	-2.228933	-1.254571
25	6	0	-2.158692	-1.980916	0.471206
26	8	0	-3.347363	-2.190014	0.257000
27	7	0	-1.499888	-0.902207	-0.098982
28	1	0	-0.983153	-1.625601	2.857036
29	6	0	-2.298207	0.106840	-0.745250
30	6	0	-3.078888	0.984421	0.037330
31	6	0	-2.285510	0.230954	-2.131895
32	6	0	-3.848632	1.964720	-0.599667
33	6	0	-3.044326	1.217857	-2.764989
34	1	0	-1.674935	-0.455588	-2.710135
35	6	0	-3.825910	2.075186	-1.992877
36	1	0	-4.458369	2.646022	-0.019321
37	1	0	-3.028071	1.307289	-3.846019
38	1	0	-4.426136	2.844098	-2.469803
39	8	0	-3.008255	0.811011	1.385079
40	6	0	-3.791133	1.665199	2.220048
41	1	0	-3.583044	1.351843	3.242970
42	1	0	-3.505660	2.715556	2.095881
43	1	0	-4.860924	1.551001	2.014134

TS18c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.152311	0.598758	-0.626227
2	6	0	-0.485396	0.176183	0.565519
3	6	0	-1.812553	-0.186303	0.509270
4	6	0	-2.558112	-0.227575	-0.695246
5	6	0	-1.871104	0.132978	-1.895852
6	6	0	-0.539723	0.505736	-1.859584
7	1	0	0.044171	0.206664	1.509325
8	6	0	-3.936733	-0.638807	-0.693227
9	1	0	-0.041187	0.788215	-2.779636
10	6	0	-4.483755	-0.977554	0.614836
11	6	0	-3.720993	-0.912037	1.732237
12	1	0	-5.521214	-1.284964	0.677633
13	6	0	-4.171725	-1.231792	3.123876
14	1	0	-5.221521	-1.532384	3.127700
15	1	0	-3.566479	-2.042632	3.545394
16	1	0	-4.047613	-0.359054	3.775058
17	8	0	-4.637758	-0.709068	-1.742304
18	8	0	-2.532730	0.087083	-3.077716
19	8	0	0.223800	2.787813	-0.394292
20	8	0	-2.419985	-0.535147	1.708852
21	6	0	1.542970	3.056595	-0.615274
22	1	0	2.038889	3.637906	0.192254
23	1	0	1.744542	3.622771	-1.552358
24	1	0	-3.458593	-0.209852	-2.866885
25	6	0	2.371162	1.773968	-0.725668
26	8	0	3.591926	1.739244	-0.859469
27	7	0	1.601699	0.620779	-0.643149
28	6	0	2.266614	-0.640075	-0.550452
29	6	0	3.011268	-0.959560	0.608815
30	6	0	2.192371	-1.570401	-1.585225
31	6	0	3.689776	-2.182117	0.684942
32	6	0	2.850316	-2.802584	-1.502084
33	1	0	1.609188	-1.315271	-2.463805
34	6	0	3.605678	-3.098821	-0.369533
35	1	0	4.273324	-2.431398	1.563764
36	1	0	2.779103	-3.512611	-2.320764
37	1	0	4.133462	-4.046029	-0.293038
38	8	0	2.992533	-0.035423	1.607840
39	6	0	3.855801	-0.207893	2.717291
40	1	0	3.719695	0.679190	3.337730
41	1	0	3.593654	-1.101617	3.300891
42	1	0	4.904194	-0.273995	2.398513
43	8	0	-0.724244	3.525799	1.962860
44	1	0	-1.548794	3.028406	2.010152
45	1	0	-0.344103	3.266606	1.063465

19c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.002958	0.680760	-0.325448
2	6	0	-0.568717	-0.463980	0.253438
3	6	0	-1.948797	-0.605318	0.226094
4	6	0	-2.796164	0.348790	-0.363292
5	6	0	-2.195964	1.496995	-0.952577
6	6	0	-0.813986	1.643633	-0.947750
7	1	0	0.046692	-1.218248	0.726651
8	6	0	-4.233856	0.149200	-0.369237
9	1	0	-0.372040	2.511304	-1.421962
10	6	0	-4.689810	-1.066073	0.269760
11	6	0	-3.813856	-1.941941	0.823296
12	1	0	-5.752101	-1.274174	0.303123
13	6	0	-4.165162	-3.221787	1.506150
14	1	0	-5.244962	-3.372307	1.508429
15	1	0	-3.687185	-4.065941	0.998272
16	1	0	-3.802768	-3.211965	2.539318
17	8	0	-5.020088	0.980060	-0.894909
18	8	0	-2.971395	2.430726	-1.538402
19	8	0	0.510571	2.725618	1.533550
20	8	0	-2.471788	-1.734601	0.809304
21	6	0	1.490517	3.077328	0.680150
22	1	0	2.395370	3.556636	1.133532
23	1	0	1.180960	3.823903	-0.101843
24	1	0	-3.909639	2.104275	-1.432707
25	6	0	2.153132	1.946869	-0.151588
26	8	0	3.313676	2.024365	-0.548392
27	7	0	1.414894	0.778899	-0.395370
28	6	0	2.124401	-0.361060	-0.905760
29	6	0	3.039673	-1.054457	-0.083696
30	6	0	1.910283	-0.797180	-2.212067
31	6	0	3.730435	-2.157603	-0.596094
32	6	0	2.588369	-1.907566	-2.720250
33	1	0	1.202220	-0.252398	-2.829065
34	6	0	3.501149	-2.578640	-1.909273
35	1	0	4.438267	-2.695520	0.022569
36	1	0	2.409995	-2.234099	-3.739580
37	1	0	4.042461	-3.439417	-2.290135
38	8	0	3.178018	-0.591182	1.190639
39	6	0	4.134271	-1.207344	2.053549
40	1	0	4.066386	-0.658032	2.992432
41	1	0	3.896826	-2.262570	2.227700
42	1	0	5.147567	-1.121712	1.647059
43	8	0	1.516877	0.972375	3.167052
44	1	0	1.825544	0.327927	2.516265
45	1	0	1.107411	1.687408	2.564367

TS19c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.581859	-0.003261	-0.040627
2	6	0	-1.866281	0.350327	0.429982
3	6	0	-2.896989	-0.571670	0.345213
4	6	0	-2.732072	-1.861611	-0.187304
5	6	0	-1.431950	-2.213456	-0.641257
6	6	0	-0.384083	-1.305448	-0.562782
7	1	0	-2.064133	1.319924	0.864881
8	6	0	-3.844187	-2.786380	-0.246981
9	1	0	0.593101	-1.619994	-0.900614
10	6	0	-5.097000	-2.275149	0.267870
11	6	0	-5.188791	-1.018506	0.770367
12	1	0	-5.971643	-2.913624	0.252111
13	6	0	-6.418867	-0.385797	1.331364
14	1	0	-7.260848	-1.077007	1.286921
15	1	0	-6.252528	-0.091096	2.372738
16	1	0	-6.669811	0.520249	0.770040
17	8	0	-3.720369	-3.950754	-0.712432
18	8	0	-1.215178	-3.445176	-1.145712
19	8	0	1.057555	1.904601	-3.084924
20	8	0	-4.126031	-0.172405	0.817345
21	6	0	1.480729	0.689635	-2.514630
22	1	0	2.332635	0.331288	-3.102590
23	1	0	0.705703	-0.082499	-2.534453
24	1	0	-2.098589	-3.911507	-1.099384
25	6	0	2.004970	0.895033	-1.091779
26	8	0	2.731155	1.791300	-0.733241
27	7	0	0.519324	0.863719	0.083953
28	6	0	0.284420	2.202218	0.531774
29	6	0	-0.489593	3.131920	-0.206240
30	6	0	0.895100	2.648631	1.708378
31	6	0	-0.669977	4.435228	0.261996
32	6	0	0.732163	3.955660	2.171964
33	1	0	1.503095	1.950006	2.272979
34	6	0	-0.058642	4.844805	1.449988
35	1	0	-0.204174	5.862486	1.798777
36	1	0	0.268299	2.190855	-2.588460
37	6	0	2.972121	-0.940184	0.456121
38	8	0	3.892467	-1.736646	0.677296
39	8	0	2.278196	-0.406149	1.449375
40	8	0	2.620942	-0.618422	-0.778937
41	1	0	1.492583	0.152629	1.021926
42	19	0	3.724256	-1.794494	3.448529
43	19	0	4.642155	-2.258488	-1.933137
44	1	0	1.215117	4.267962	3.092360
45	1	0	-1.273046	5.138916	-0.298351
46	8	0	-1.033904	2.676122	-1.383294
47	6	0	-2.031477	3.475366	-2.033608
48	1	0	-2.388984	2.875884	-2.870351
49	1	0	-2.859214	3.689554	-1.351231
50	1	0	-1.609715	4.412648	-2.410080

14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.925369	0.054563	-0.522743
2	6	0	2.278348	0.448129	-0.494698

3	6	0	3.250943	-0.536205	-0.419385
4	6	0	2.954974	-1.911102	-0.377272
5	6	0	1.580676	-2.288205	-0.420976
6	6	0	0.589779	-1.322253	-0.492245
7	1	0	2.570594	1.488242	-0.540714
8	6	0	4.013778	-2.892106	-0.301090
9	1	0	-0.450189	-1.625655	-0.526054
10	6	0	5.356931	-2.350106	-0.274905
11	6	0	5.574638	-1.012952	-0.323077
12	1	0	6.197235	-3.031075	-0.219209
13	6	0	6.905535	-0.337161	-0.307946
14	1	0	7.709048	-1.072068	-0.252326
15	1	0	7.035081	0.266290	-1.212431
16	1	0	6.978835	0.338443	0.550664
17	8	0	3.778866	-4.130703	-0.263255
18	8	0	1.251983	-3.594909	-0.389247
19	8	0	-0.902239	1.194411	3.280891
20	8	0	4.558275	-0.111948	-0.393038
21	6	0	-1.391665	0.017928	2.694058
22	1	0	-1.899538	-0.567495	3.469155
23	1	0	-0.598791	-0.621649	2.279398
24	1	0	2.122124	-4.087125	-0.334804
25	6	0	-2.387524	0.296151	1.573784
26	8	0	-2.803780	1.388777	1.263137
27	7	0	-0.107966	0.965101	-0.583863
28	6	0	0.030683	2.370608	-0.689369
29	6	0	0.586058	3.139963	0.359193
30	6	0	-0.452171	3.031166	-1.823747
31	6	0	0.697554	4.526641	0.225466
32	6	0	-0.372969	4.419390	-1.943087
33	1	0	-0.881478	2.433790	-2.622733
34	6	0	0.216807	5.162067	-0.922368
35	1	0	0.302222	6.240937	-1.006374
36	1	0	-0.385068	1.659146	2.597572
37	6	0	-3.403120	-0.772084	-0.356060
38	8	0	-4.488051	-1.371970	-0.399982
39	8	0	-2.753031	-0.187980	-1.235769
40	8	0	-2.751334	-0.860784	0.959274
41	1	0	-1.018162	0.589826	-0.861183
42	19	0	-4.768054	-0.617957	-3.099219
43	19	0	-4.744574	-2.848809	1.850192
44	1	0	-0.751530	4.909296	-2.834322
45	1	0	1.135996	5.118384	1.019620
46	8	0	0.973814	2.451949	1.483170
47	6	0	1.795412	3.126846	2.445609
48	1	0	2.058749	2.371854	3.185872
49	1	0	2.702110	3.517961	1.974680
50	1	0	1.252212	3.941351	2.935437

5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.025234	0.607741	0.000039
2	1	0	-4.479029	1.047315	-0.887864
3	1	0	-4.478772	1.047468	0.887997
4	6	0	-2.533847	0.955436	-0.000167
5	8	0	-2.256228	2.151977	-0.000310
6	7	0	-1.651140	-0.074373	-0.000189
7	17	0	-4.466114	-1.156652	0.000237
8	1	0	-2.056660	-1.002106	-0.000012
9	6	0	-0.238095	-0.031427	-0.000129
10	6	0	0.422783	-1.266153	-0.000175
11	6	0	1.819084	-1.299904	-0.000087
12	6	0	1.883242	1.106799	0.000093
13	6	0	2.568919	-0.114990	0.000052
14	1	0	3.648179	-0.144172	0.000115
15	1	0	-0.127213	-2.201186	-0.000280
16	8	0	2.507084	2.320216	0.000199
17	8	0	2.371928	-2.546671	-0.000143
18	6	0	3.932537	2.356525	0.000119
19	1	0	4.203921	3.412474	0.000122
20	1	0	4.346897	1.876553	0.894113
21	1	0	4.346813	1.876562	-0.893919
22	6	0	3.793303	-2.663594	0.000056
23	1	0	4.233621	-2.207990	0.894255
24	1	0	4.004106	-3.733242	0.000003
25	1	0	4.233879	-2.207834	-0.893941
26	6	0	0.484024	1.165324	-0.000009
27	1	0	-0.016388	2.121144	-0.000017

TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.906290	-1.095969	-0.748381
2	6	0	2.378873	-0.220751	0.275885
3	6	0	3.635701	0.340152	0.157732
4	6	0	4.494823	0.100232	-0.937090
5	6	0	4.013103	-0.767929	-1.965480
6	6	0	2.762000	-1.348329	-1.867476
7	1	0	1.743300	0.033932	1.115085
8	6	0	5.794453	0.715471	-1.004460
9	1	0	2.412873	-2.013118	-2.650510
10	6	0	6.132579	1.577659	0.112622
11	6	0	5.263773	1.774474	1.133510
12	1	0	7.096917	2.070943	0.121809
13	6	0	5.495175	2.637385	2.330679
14	1	0	6.477823	3.107759	2.282007
15	1	0	4.728965	3.417448	2.391665
16	1	0	5.429630	2.042233	3.247673
17	8	0	6.589028	0.522018	-1.969458
18	8	0	4.805336	-1.021564	-3.032115
19	8	0	0.736090	-1.662500	-0.710955
20	8	0	4.041946	1.181588	1.174458
21	6	0	-0.057418	-2.244692	1.134540
22	1	0	0.906564	-2.088820	1.586089
23	1	0	-0.239651	-3.151424	0.584739
24	1	0	5.644011	-0.501379	-2.866934
25	6	0	-0.979612	-1.063751	1.057807
26	8	0	-0.710249	-0.001829	1.615432
27	7	0	-2.116594	-1.299413	0.331334
28	17	0	-0.893802	-3.132434	3.018023
29	1	0	-2.194962	-2.218352	-0.081167
30	6	0	-3.193126	-0.433610	0.058699
31	6	0	-4.232250	-0.951666	-0.727853
32	6	0	-3.254847	0.879968	0.537207
33	6	0	-5.334755	-0.151339	-1.032472
34	6	0	-4.370755	1.663090	0.219248
35	1	0	-2.460989	1.290017	1.141494
36	6	0	-5.421478	1.167460	-0.563724
37	1	0	-6.275443	1.784162	-0.800074
38	1	0	-4.199692	-1.968121	-1.105999
39	8	0	-4.346228	2.929705	0.729465
40	8	0	-6.292759	-0.745922	-1.802112
41	6	0	-5.445826	3.795602	0.460361
42	1	0	-5.214791	4.736274	0.961051
43	1	0	-5.561541	3.977119	-0.614425
44	1	0	-6.382746	3.392712	0.862194
45	6	0	-7.453625	0.006095	-2.147225
46	1	0	-7.197320	0.895243	-2.734621
47	1	0	-8.070917	-0.658726	-2.752033
48	1	0	-8.015003	0.310089	-1.256285

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.867355	1.375475	0.379730
2	6	0	2.124754	0.566717	-0.733004
3	6	0	3.131657	-0.388170	-0.611501
4	6	0	3.877824	-0.566523	0.562351
5	6	0	3.583525	0.272534	1.676295
6	6	0	2.585553	1.234141	1.578402
7	1	0	1.576223	0.640995	-1.661564
8	6	0	4.913999	-1.582458	0.626843
9	1	0	2.361327	1.879344	2.419360
10	6	0	5.092630	-2.357331	-0.581150
11	6	0	4.331515	-2.130380	-1.680626
12	1	0	5.849059	-3.131993	-0.600666
13	6	0	4.419992	-2.860502	-2.978666
14	1	0	5.195970	-3.625046	-2.936364
15	1	0	3.461369	-3.335121	-3.212300
16	1	0	4.648170	-2.162709	-3.790964
17	8	0	5.599572	-1.766009	1.665445
18	8	0	4.276569	0.132260	2.818207
19	8	0	0.908832	2.348486	0.403883
20	8	0	3.368039	-1.171062	-1.711282
21	6	0	0.198798	2.667634	-0.797362
22	1	0	0.864554	2.705100	-1.663186
23	1	0	-0.214797	3.671950	-0.629373
24	1	0	4.929101	-0.607134	2.648775
25	6	0	-0.957770	1.715791	-1.114475
26	8	0	-1.401732	1.655879	-2.258594
27	7	0	-1.437592	1.041447	-0.030864
28	17	0	-1.065450	6.038338	-0.015443
29	1	0	-0.949698	1.229797	0.836421
30	6	0	-2.506799	0.124970	0.052608
31	6	0	-2.765417	-0.426304	1.314332
32	6	0	-3.284267	-0.231930	-1.053794
33	6	0	-3.810384	-1.340060	1.466700
34	6	0	-4.325842	-1.150726	-0.877057
35	1	0	-3.093120	0.189025	-2.028781
36	6	0	-4.605188	-1.715724	0.374283
37	1	0	-5.412861	-2.421779	0.495376
38	1	0	-2.169586	-0.157359	2.180060
39	8	0	-5.032257	-1.442018	-2.008388
40	8	0	-3.985151	-1.821051	2.731630
41	6	0	-6.114526	-2.365458	-1.919453
42	1	0	-6.524515	-2.442667	-2.926816
43	1	0	-5.773876	-3.354170	-1.590969
44	1	0	-6.894466	-2.006326	-1.238181
45	6	0	-5.033313	-2.758696	2.966313
46	1	0	-4.892205	-3.674108	2.380362
47	1	0	-4.985100	-3.000185	4.028422
48	1	0	-6.015306	-2.329345	2.737150

TS17d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.687526	2.134905	-0.458617
2	6	0	1.577521	1.251533	-1.175885
3	6	0	2.318942	0.319342	-0.496123
4	6	0	2.325809	0.197897	0.917961
5	6	0	1.515008	1.137918	1.643120
6	6	0	0.770097	2.088729	0.993517
7	1	0	1.628966	1.317321	-2.256146
8	6	0	3.134113	-0.775692	1.572710
9	1	0	0.189500	2.794294	1.579299
10	6	0	3.923120	-1.627453	0.692141
11	6	0	3.886421	-1.469983	-0.650438
12	1	0	4.555020	-2.391651	1.128955
13	6	0	4.652832	-2.270287	-1.653317
14	1	0	5.272125	-3.017755	-1.155726
15	1	0	3.969193	-2.777322	-2.342889
16	1	0	5.296557	-1.618038	-2.253374
17	8	0	3.182531	-0.902203	2.837894
18	8	0	1.532799	1.082240	3.000192
19	8	0	0.641080	3.426521	-1.051511
20	8	0	3.112822	-0.524967	-1.254002
21	6	0	-0.620432	4.055505	-0.896528
22	1	0	-0.766381	4.748208	-1.730792
23	1	0	-0.688466	4.632430	0.038845
24	1	0	2.155453	0.327368	3.219025
25	6	0	-1.694802	2.969086	-0.886452
26	8	0	-2.906087	3.241708	-0.880444
27	7	0	-1.072080	1.783254	-0.882569
28	6	0	-1.692680	0.558390	-0.608335
29	6	0	-1.251452	-0.586525	-1.289347
30	6	0	-2.700357	0.439884	0.363874
31	6	0	-1.811879	-1.832592	-0.995420
32	6	0	-3.260622	-0.810021	0.634615
33	1	0	-3.063537	1.312328	0.891033
34	6	0	-2.824160	-1.963774	-0.034340
35	1	0	-3.260289	-2.927517	0.182675
36	1	0	-0.477053	-0.512447	-2.041996
37	8	0	-1.309937	-2.885880	-1.712419
38	8	0	-4.243371	-0.819177	1.589167
39	6	0	-1.835648	-4.186384	-1.468958
40	1	0	-1.295180	-4.858527	-2.136566
41	1	0	-1.671983	-4.500819	-0.431378
42	1	0	-2.907233	-4.238668	-1.695711
43	6	0	-4.844406	-2.062620	1.934717
44	1	0	-4.107737	-2.770960	2.332102
45	1	0	-5.578471	-1.836469	2.709069
46	1	0	-5.354339	-2.517637	1.077170

18d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.49446800	1.99964300	-0.33292800
2	6	0	1.23097500	0.94928700	-1.13233200
3	6	0	2.11526000	0.09648400	-0.52399900
4	6	0	2.35329500	0.13438800	0.86940000
5	6	0	1.66660300	1.09161400	1.70995300
6	6	0	0.78314700	1.96674500	1.14445000
7	1	0	1.12761800	0.96967400	-2.21076700
8	6	0	3.31940100	-0.82149700	1.45361300
9	1	0	0.25477600	2.68505100	1.76081000
10	6	0	3.93987000	-1.71178000	0.51383100
11	6	0	3.65534600	-1.66918900	-0.82047300
12	1	0	4.65646500	-2.43420800	0.88301700
13	6	0	4.24581300	-2.54192900	-1.86908300
14	1	0	4.96113000	-3.23821300	-1.43315800
15	1	0	3.45361700	-3.10329400	-2.37524600
16	1	0	4.74835700	-1.92862400	-2.62406600
17	8	0	3.54993000	-0.82494800	2.68026900
18	8	0	1.89934500	1.11377800	3.02694800
19	8	0	0.85647600	3.28412600	-0.86341000
20	8	0	2.76700800	-0.78801600	-1.33515600
21	6	0	-0.31384800	4.01432300	-1.25311800
22	1	0	-0.20574800	4.35280400	-2.28710700
23	1	0	-0.46234300	4.88024300	-0.59896100
24	1	0	2.56769400	0.40056700	3.21877000
25	6	0	-1.47757900	3.04632500	-1.12778400
26	8	0	-2.63916700	3.22846500	-1.43517800
27	7	0	-0.94977400	1.89435800	-0.58604900
28	6	0	-1.65094100	0.66617100	-0.36831800
29	6	0	-1.37848800	-0.41382500	-1.21888100
30	6	0	-2.54485800	0.55213900	0.68097600
31	6	0	-1.98955900	-1.66027200	-0.95663400
32	6	0	-3.18254200	-0.69076800	0.90274300
33	1	0	-2.74533600	1.38042600	1.34883500
34	6	0	-2.89500600	-1.80329900	0.10136100
35	1	0	-3.37324100	-2.75285600	0.28960200
36	1	0	-0.81273100	-0.29562700	-2.13292500
37	8	0	-1.65634500	-2.64740800	-1.81049100
38	8	0	-4.03864000	-0.70698200	1.94064200
39	6	0	-2.26020000	-3.93809100	-1.65524600
40	1	0	-1.84374300	-4.55337800	-2.45136500
41	1	0	-2.00882900	-4.37385300	-0.68321600
42	1	0	-3.34723800	-3.87705600	-1.76632300
43	6	0	-4.70740600	-1.92873700	2.28069500
44	1	0	-3.98647600	-2.70684800	2.54965900
45	1	0	-5.32978300	-1.69099500	3.14196500
46	1	0	-5.33713900	-2.27283900	1.45447100

TS18d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.456487	1.188545	0.263666
2	6	0	1.328835	0.674295	-0.757235
3	6	0	2.372968	-0.147149	-0.401054
4	6	0	2.573994	-0.620214	0.918617
5	6	0	1.618663	-0.209190	1.904957
6	6	0	0.569215	0.620080	1.576735
7	1	0	1.201161	0.983615	-1.788179
8	6	0	3.658275	-1.502592	1.227975
9	1	0	-0.149480	0.903212	2.337689
10	6	0	4.519935	-1.848514	0.108046
11	6	0	4.282015	-1.367725	-1.134330
12	1	0	5.361441	-2.509132	0.278771
13	6	0	5.086772	-1.654896	-2.359818
14	1	0	5.918115	-2.321205	-2.126537
15	1	0	4.460656	-2.122285	-3.127382
16	1	0	5.483471	-0.725815	-2.782963
17	8	0	3.859991	-1.961953	2.392882
18	8	0	1.753998	-0.676387	3.169441
19	8	0	0.970430	2.995265	0.482719
20	8	0	3.239712	-0.535078	-1.407108
21	6	0	0.070240	3.730160	-0.264338
22	1	0	0.472838	4.093138	-1.230676
23	1	0	-0.313734	4.623506	0.262275
24	1	0	2.569717	-1.257373	3.146933
25	6	0	-1.140522	2.857488	-0.569206
26	8	0	-2.177729	3.260864	-1.088206
27	7	0	-0.900835	1.564962	-0.160759
28	6	0	-1.919484	0.562705	-0.201712
29	6	0	-1.635309	-0.716241	-0.688836
30	6	0	-3.199146	0.868278	0.273028
31	6	0	-2.641101	-1.688206	-0.698142
32	6	0	-4.196774	-0.109929	0.240884

33	1	0	-3.435702	1.851959	0.654510
34	6	0	-3.933254	-1.400353	-0.239797
35	1	0	-4.706708	-2.153881	-0.254612
36	1	0	-0.649249	-0.969369	-1.055059
37	8	0	-2.266583	-2.907930	-1.188074
38	8	0	-5.415579	0.284549	0.717459
39	6	0	-3.239329	-3.947862	-1.239817
40	1	0	-2.728633	-4.814668	-1.660360
41	1	0	-3.613805	-4.198785	-0.240555
42	1	0	-4.083646	-3.677732	-1.884760
43	6	0	-6.478362	-0.664314	0.736993
44	1	0	-6.237361	-1.526120	1.370206
45	1	0	-7.339012	-0.140883	1.154546
46	1	0	-6.723817	-1.014884	-0.272284
47	8	0	3.289773	3.359514	-0.856874
48	1	0	3.375736	2.517190	-1.320585
49	1	0	2.487054	3.207812	-0.293278

19d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.394350	0.580921	0.189401
2	6	0	1.453925	0.548521	-0.725969
3	6	0	2.572780	-0.206004	-0.407898
4	6	0	2.657284	-0.982479	0.761261
5	6	0	1.546281	-0.970610	1.650059
6	6	0	0.427390	-0.198077	1.356732
7	1	0	1.418637	1.113970	-1.648502
8	6	0	3.846514	-1.768656	1.035541
9	1	0	-0.408488	-0.187415	2.046244
10	6	0	4.889300	-1.679437	0.036026
11	6	0	4.741533	-0.907592	-1.069443
12	1	0	5.803123	-2.242356	0.180499
13	6	0	5.743468	-0.735757	-2.161956
14	1	0	6.634529	-1.331671	-1.963272
15	1	0	5.314164	-1.041837	-3.121564
16	1	0	6.029858	0.317363	-2.251015
17	8	0	3.953241	-2.475575	2.071176
18	8	0	1.583633	-1.703932	2.778697
19	8	0	1.156210	3.104837	0.868998
20	8	0	3.617229	-0.179853	-1.302800
21	6	0	0.407031	3.507592	-0.178524
22	1	0	0.959761	3.590620	-1.153461
23	1	0	-0.069112	4.515337	-0.076879
24	1	0	2.473866	-2.157704	2.774699
25	6	0	-0.824774	2.635652	-0.524810
26	8	0	-1.816691	3.104259	-1.078983
27	7	0	-0.802340	1.291470	-0.126847
28	6	0	-2.014397	0.522177	-0.189250
29	6	0	-2.042405	-0.655677	-0.938366
30	6	0	-3.142564	0.945557	0.515292
31	6	0	-3.215299	-1.417662	-0.976694
32	6	0	-4.313440	0.183404	0.454222
33	1	0	-3.127771	1.855747	1.101215
34	6	0	-4.363581	-1.006850	-0.286239
35	1	0	-5.268139	-1.595493	-0.321755
36	1	0	-1.171273	-0.991263	-1.488355
37	8	0	-3.149507	-2.555592	-1.728360
38	8	0	-5.369482	0.674328	1.167220
39	6	0	-4.311277	-3.375884	-1.826355
40	1	0	-4.032666	-4.213044	-2.466948
41	1	0	-4.617835	-3.757515	-0.845642
42	1	0	-5.148388	-2.834593	-2.282124
43	6	0	-6.590170	-0.061804	1.172782
44	1	0	-6.454092	-1.063407	1.596866
45	1	0	-7.277625	0.504729	1.801487
46	1	0	-7.011682	-0.149709	0.164748
47	8	0	3.551598	3.194089	-0.046940
48	1	0	3.580450	2.453085	-0.663331
49	1	0	2.607518	3.130359	0.358076

TS19d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.919761	0.559829	0.069921
2	6	0	-1.948101	-0.392512	0.063635
3	6	0	-3.259447	0.048611	-0.078358
4	6	0	-3.597464	1.402549	-0.210583
5	6	0	-2.539634	2.351005	-0.200926
6	6	0	-1.219633	1.928741	-0.070375
7	1	0	-1.751187	-1.450084	0.163296
8	6	0	-4.987199	1.805841	-0.355652
9	1	0	-0.436435	2.673353	-0.061802
10	6	0	-5.943637	0.722120	-0.346997
11	6	0	-5.543640	-0.568051	-0.213629
12	1	0	-6.997282	0.950185	-0.449315
13	6	0	-6.433961	-1.765065	-0.190160
14	1	0	-7.477761	-1.469361	-0.297166
15	1	0	-6.169740	-2.449089	-1.003198
16	1	0	-6.310299	-2.309994	0.751403
17	8	0	-5.315915	3.013042	-0.478074
18	8	0	-2.812405	3.660905	-0.328697
19	8	0	0.578778	-0.020873	3.539013
20	8	0	-4.236138	-0.914796	-0.082765
21	6	0	0.521792	1.113773	2.691134
22	1	0	0.951550	2.000832	3.178072
23	1	0	-0.522498	1.325833	2.461380
24	1	0	-3.806755	3.722572	-0.413208
25	6	0	1.382358	0.840230	1.439957
26	8	0	2.438091	0.176901	1.625381
27	7	0	0.463636	0.172611	0.181468
28	6	0	0.737428	-1.245713	-0.010465
29	6	0	0.604991	-2.160560	1.033492
30	6	0	1.108530	-1.663810	-1.287851
31	6	0	0.860250	-3.514441	0.788063
32	6	0	1.355711	-3.022887	-1.521590
33	1	0	1.201074	-0.963032	-2.109288
34	6	0	1.235620	-3.960206	-0.488028
35	1	0	1.429570	-5.006866	-0.669884
36	1	0	0.328363	-1.833732	2.028049
37	1	0	1.480429	-0.365433	3.400611
38	6	0	2.333699	2.347168	-0.287462
39	8	0	3.253331	3.160020	-0.412537
40	8	0	1.924318	1.556778	-1.241295
41	8	0	1.678793	2.255704	0.897151
42	1	0	1.162470	0.844154	-0.727591
43	19	0	3.751213	2.601193	-3.117904
44	19	0	4.409779	2.064862	2.068529
45	8	0	1.711898	-3.341660	-2.798724
46	8	0	0.718186	-4.340071	1.864360
47	6	0	0.949158	-5.736675	1.690178
48	1	0	0.777428	-6.191229	2.666050
49	1	0	0.254793	-6.170412	0.961573
50	1	0	1.979273	-5.936683	1.373866
51	6	0	1.966662	-4.709447	-3.114904
52	1	0	1.081017	-5.331552	-2.942946
53	1	0	2.220354	-4.728142	-4.174893
54	1	0	2.807504	-5.105264	-2.534067

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.251261	-0.197826	-0.296933
2	6	0	2.537716	0.374563	-0.376950
3	6	0	3.639555	-0.466734	-0.331884
4	6	0	3.539650	-1.864218	-0.218479
5	6	0	2.230564	-2.424954	-0.155704
6	6	0	1.114449	-1.604760	-0.191554
7	1	0	2.686812	1.437167	-0.502551
8	6	0	4.726929	-2.689262	-0.179402
9	1	0	0.127109	-2.047209	-0.128759
10	6	0	5.980691	-1.969823	-0.267617
11	6	0	6.007706	-0.619088	-0.382626
12	1	0	6.909101	-2.527008	-0.244744
13	6	0	7.230294	0.230744	-0.486564
14	1	0	8.129711	-0.384713	-0.455242
15	1	0	7.218706	0.799782	-1.422029
16	1	0	7.261697	0.952497	0.336264
17	8	0	4.666329	-3.944698	-0.079946
18	8	0	2.086950	-3.760416	-0.050945
19	8	0	-2.255895	-0.013776	3.990674
20	8	0	4.873897	0.131451	-0.415426
21	6	0	-1.911764	-1.044197	3.095034
22	1	0	-2.200512	-2.014255	3.514601
23	1	0	-0.827644	-1.085474	2.900160
24	1	0	3.017970	-4.128344	-0.037146
25	6	0	-2.600537	-0.848678	1.755642
26	8	0	-3.187817	0.176778	1.468945
27	7	0	0.086343	0.539556	-0.357773
28	6	0	-0.102263	1.926381	-0.256060
29	6	0	0.711328	2.750135	0.534195
30	6	0	-1.204963	2.475558	-0.928536
31	6	0	0.429492	4.118101	0.620067
32	6	0	-1.480612	3.839698	-0.815299
33	1	0	-1.851046	1.850042	-1.534089
34	6	0	-0.662877	4.684556	-0.050258
35	1	0	-0.872387	5.740827	0.024457
36	1	0	1.533105	2.353567	1.115085
37	1	0	-2.569316	0.721475	3.437787
38	6	0	-2.934754	-1.785994	-0.457409
39	8	0	-3.863987	-2.558105	-0.721756
40	8	0	-2.284540	-0.996949	-1.152924
41	8	0	-2.471247	-1.915744	0.952184
42	1	0	-0.752545	0.007420	-0.596408
43	19	0	-3.823192	-1.617017	-3.397156
44	19	0	-4.191549	-4.365313	1.283609
45	8	0	-2.577433	4.272836	-1.504452
46	8	0	1.282775	4.833751	1.410392
47	6	0	1.046377	6.228949	1.582613
48	1	0	1.832258	6.584810	2.249423
49	1	0	1.109192	6.767875	0.630265
50	1	0	0.069159	6.417664	2.041755

51	6	0	-2.918873	5.655897	-1.444502
52	1	0	-2.119900	6.285472	-1.852665
53	1	0	-3.814016	5.769354	-2.056547
54	1	0	-3.140225	5.971111	-0.418409

6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.211930	0.799379	-0.131296
2	1	0	-3.673617	0.921518	-1.110869
3	1	0	-3.774747	1.375707	0.602658
4	6	0	-1.792303	1.366998	-0.198124
5	8	0	-1.689926	2.548385	-0.509627
6	7	0	-0.765187	0.519938	0.088595
7	17	0	-3.382326	-0.950468	0.324244
8	1	0	-1.030883	-0.428069	0.324521
9	6	0	0.616773	0.811754	0.093855
10	6	0	1.549368	-0.250587	0.040363
11	6	0	1.094416	2.126837	0.180775
12	6	0	2.918967	0.018960	0.080735
13	6	0	2.465564	2.375508	0.213754
14	1	0	0.386469	2.941470	0.216420
15	6	0	3.384686	1.328519	0.168879
16	1	0	3.617904	-0.807515	0.038778
17	1	0	2.811964	3.401972	0.283059
18	1	0	4.450847	1.525080	0.199299
19	6	0	1.093551	-1.674721	-0.119870
20	9	0	2.105066	-2.557376	-0.045150
21	9	0	0.469467	-1.878099	-1.305550
22	9	0	0.189108	-2.032829	0.841410

TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.547606	-1.055658	0.155253
2	6	0	2.186517	0.215868	0.261278
3	6	0	3.538383	0.316013	-0.005897
4	6	0	4.338670	-0.783247	-0.386157
5	6	0	3.692398	-2.053267	-0.497941
6	6	0	2.341691	-2.181243	-0.230005
7	1	0	1.611315	1.099641	0.508495
8	6	0	5.743413	-0.615765	-0.654735
9	1	0	1.865567	-3.152770	-0.309798
10	6	0	6.246758	0.737254	-0.509549
11	6	0	5.427994	1.754102	-0.146898
12	1	0	7.295627	0.930438	-0.698920
13	6	0	5.826612	3.182891	0.029041
14	1	0	6.890035	3.313191	-0.174275
15	1	0	5.252848	3.824311	-0.648240
16	1	0	5.615322	3.514453	1.051147
17	8	0	6.489323	-1.578249	-0.996203
18	8	0	4.424694	-3.130831	-0.860104
19	8	0	0.277702	-1.230172	0.384069
20	8	0	4.105385	1.569998	0.104003
21	6	0	-0.636081	-0.132211	1.900744
22	1	0	0.331157	0.179974	2.253824
23	1	0	-1.003491	-1.107893	2.166152
24	1	0	5.355365	-2.786123	-0.987864
25	6	0	-1.276171	0.699919	0.831002
26	8	0	-0.803666	1.777985	0.483659
27	7	0	-2.422490	0.140910	0.315299
28	17	0	-1.681258	0.817208	3.643359
29	1	0	-2.662190	-0.768627	0.681896
30	6	0	-3.260013	0.639780	-0.696797
31	6	0	-4.515628	0.023577	-0.926358
32	6	0	-2.887371	1.722393	-1.510306
33	6	0	-5.349871	0.487405	-1.945950
34	6	0	-3.737494	2.172010	-2.518505
35	1	0	-1.934349	2.199347	-1.337948
36	6	0	-4.968607	1.559376	-2.748472
37	1	0	-6.305282	0.001578	-2.103062
38	1	0	-3.423291	3.009693	-3.133739
39	1	0	-5.625466	1.910032	-3.537082
40	6	0	-5.004391	-1.092477	-0.046484
41	9	0	-6.153485	-1.638735	-0.483323
42	9	0	-5.216125	-0.681521	1.228607
43	9	0	-4.096874	-2.112668	0.041631

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.812474	1.467690	0.423586
2	6	0	1.384131	1.037832	-0.778949
3	6	0	2.633676	0.425691	-0.711088
4	6	0	3.322416	0.227610	0.494102
5	6	0	2.706171	0.675543	1.698647
6	6	0	1.460693	1.289727	1.656381
7	1	0	0.901742	1.146541	-1.740263
8	6	0	4.622669	-0.420122	0.498714
9	1	0	0.988557	1.635476	2.568075
10	6	0	5.114290	-0.823258	-0.800200
11	6	0	4.391468	-0.599889	-1.925859
12	1	0	6.077972	-1.312535	-0.867798
13	6	0	4.789454	-0.968426	-3.315676
14	1	0	5.764908	-1.455259	-3.319173
15	1	0	4.049429	-1.645572	-3.754586
16	1	0	4.832788	-0.074874	-3.946951
17	8	0	5.264872	-0.611634	1.563218
18	8	0	3.334799	0.503324	2.872909
19	8	0	-0.406675	2.081315	0.506619
20	8	0	3.176180	0.010083	-1.898948
21	6	0	-1.122523	2.389263	-0.693589
22	1	0	-0.468981	2.810387	-1.461421
23	1	0	-1.859987	3.152940	-0.406335
24	1	0	4.198417	0.048580	2.652637
25	6	0	-1.868549	1.194775	-1.291227
26	8	0	-2.207263	1.203211	-2.469869
27	7	0	-2.137173	0.206794	-0.382549
28	17	0	-3.488078	4.987156	0.305374
29	1	0	-1.789116	0.395341	0.549060
30	6	0	-2.789033	-1.023586	-0.588014
31	6	0	-2.663900	-2.043692	0.385067
32	6	0	-3.574178	-1.266601	-1.724458
33	6	0	-3.322038	-3.262605	0.210752
34	6	0	-4.217664	-2.492798	-1.883175
35	1	0	-3.665525	-0.491536	-2.471033
36	6	0	-4.101755	-3.494362	-0.919961
37	1	0	-3.214485	-4.030886	0.966956
38	1	0	-4.821597	-2.658198	-2.770073
39	1	0	-4.608156	-4.445249	-1.045349
40	6	0	-1.788268	-1.848689	1.591102
41	9	0	-1.828935	-2.888273	2.442657
42	9	0	-2.145603	-0.739526	2.305199
43	9	0	-0.487786	-1.658798	1.250408

TS17e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.017654	-1.408682	-1.028839
2	6	0	-0.693391	-0.205312	-1.461337
3	6	0	-1.875411	0.167718	-0.877778
4	6	0	-2.553017	-0.607443	0.100819
5	6	0	-1.938137	-1.854364	0.462400
6	6	0	-0.753206	-2.256612	-0.101128
7	1	0	-0.221538	0.422272	-2.205461
8	6	0	-3.795179	-0.181912	0.652843
9	1	0	-0.333049	-3.217058	0.180696
10	6	0	-4.296174	1.093114	0.155738
11	6	0	-3.616249	1.794633	-0.779365
12	1	0	-5.234260	1.474678	0.541073
13	6	0	-4.027447	3.103537	-1.372191
14	1	0	-4.974182	3.438579	-0.946381
15	1	0	-3.263833	3.866063	-1.184150
16	1	0	-4.138339	3.014462	-2.458349
17	8	0	-4.440484	-0.858881	1.515976
18	8	0	-2.579376	-2.645929	1.360480
19	8	0	0.619998	-2.078708	-2.115348
20	8	0	-2.434159	1.362900	-1.300815
21	6	0	1.814776	-2.738755	-1.727896
22	1	0	2.481737	-2.781967	-2.594060
23	1	0	1.634089	-3.768965	-1.384893
24	1	0	-3.410738	-2.139230	1.602140
25	6	0	2.443257	-1.937119	-0.589171
26	8	0	3.552999	-2.203699	-0.107664
27	7	0	1.566333	-0.984427	-0.250212
28	6	0	1.688264	-0.159960	0.874286
29	6	0	2.213295	1.149744	0.775252
30	6	0	1.230829	-0.598731	2.127987
31	6	0	2.267412	1.975006	1.902112
32	6	0	1.281093	0.233639	3.245120
33	1	0	0.830638	-1.602911	2.205633
34	6	0	1.798688	1.524639	3.135671
35	1	0	2.679868	2.972804	1.810796
36	1	0	0.919475	-0.129824	4.202572
37	1	0	1.843878	2.176234	4.002284
38	6	0	2.741408	1.667129	-0.536659
39	9	0	1.777537	1.790248	-1.482717
40	9	0	3.300022	2.896671	-0.406484
41	9	0	3.699239	0.868499	-1.065091

18e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.012000	-1.214370	-0.834221
2	6	0	-0.673874	0.063850	-1.155478
3	6	0	-1.928895	0.343231	-0.702659
4	6	0	-2.701054	-0.528121	0.120658
5	6	0	-2.075953	-1.778324	0.470902

6	6	0	-0.816988	-2.097370	0.047057
7	1	0	-0.144832	0.773493	-1.776912
8	6	0	-4.000475	-0.177566	0.560266
9	1	0	-0.391109	-3.056022	0.331300
10	6	0	-4.483841	1.126864	0.114124
11	6	0	-3.721180	1.924555	-0.665030
12	1	0	-5.471948	1.452592	0.417600
13	6	0	-4.099946	3.274451	-1.184470
14	1	0	-5.101840	3.548128	-0.850410
15	1	0	-3.390796	4.033663	-0.836437
16	1	0	-4.076284	3.285814	-2.279756
17	8	0	-4.722701	-0.931995	1.296610
18	8	0	-2.786340	-2.640017	1.250087
19	8	0	0.352875	-1.905877	-2.101338
20	8	0	-2.471598	1.567124	-1.077941
21	6	0	1.566175	-2.611475	-1.937462
22	1	0	2.163054	-2.553635	-2.854743
23	1	0	1.419043	-3.676138	-1.695183
24	1	0	-3.656687	-2.168381	1.422555
25	6	0	2.295844	-1.934060	-0.786028
26	8	0	3.429955	-2.194809	-0.394057
27	7	0	1.426013	-1.014225	-0.288001
28	6	0	1.710510	-0.225082	0.859324
29	6	0	2.458329	0.968247	0.762444
30	6	0	1.245304	-0.630594	2.115223
31	6	0	2.720505	1.718248	1.913153
32	6	0	1.501413	0.131232	3.255208
33	1	0	0.673258	-1.547699	2.181117
34	6	0	2.242619	1.307008	3.156422
35	1	0	3.299564	2.629596	1.830830
36	1	0	1.128627	-0.202308	4.218736
37	1	0	2.452685	1.902408	4.038925
38	6	0	2.984011	1.474206	-0.559399
39	9	0	1.993700	1.750390	-1.443160
40	9	0	3.688064	2.622022	-0.411331
41	9	0	3.810974	0.595708	-1.169811

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.153047	0.839297	-0.601438
2	6	0	0.748756	-0.460276	-0.498424
3	6	0	2.084421	-0.567806	-0.190506
4	6	0	2.905679	0.537937	0.138709
5	6	0	2.276737	1.824869	0.148618
6	6	0	0.940433	1.961426	-0.153804
7	1	0	0.171606	-1.341591	-0.737626
8	6	0	4.283092	0.359543	0.484393
9	1	0	0.489091	2.948083	-0.125941
10	6	0	4.760046	-1.014063	0.454189
11	6	0	3.931686	-2.035455	0.133619
12	1	0	5.795688	-1.215947	0.699893
13	6	0	4.300707	-3.482068	0.072591
14	1	0	5.351042	-3.622279	0.330809
15	1	0	3.683027	-4.063940	0.765042
16	1	0	4.125614	-3.878539	-0.933272
17	8	0	5.042967	1.324885	0.801524
18	8	0	3.018413	2.905868	0.492762
19	8	0	-0.126175	1.145758	-2.427999
20	8	0	2.622324	-1.842036	-0.181704
21	6	0	-1.307242	1.868605	-2.496449
22	1	0	-1.977827	1.515343	-3.298917
23	1	0	-1.167703	2.954475	-2.656394
24	1	0	3.933034	2.543330	0.681922
25	6	0	-2.064887	1.685009	-1.185181
26	8	0	-3.181829	2.120407	-0.931255
27	7	0	-1.298986	0.914548	-0.337510
28	6	0	-1.796869	0.553293	0.954155
29	6	0	-2.693638	-0.524390	1.112996
30	6	0	-1.404208	1.279053	2.082273
31	6	0	-3.177910	-0.840888	2.386453
32	6	0	-1.883885	0.948935	3.349481
33	1	0	-0.711815	2.102554	1.954089
34	6	0	-2.777832	-0.109050	3.502990
35	1	0	-3.866493	-1.668772	2.501091
36	1	0	-1.564648	1.526393	4.211424
37	1	0	-3.161913	-0.368728	4.483907
38	6	0	-3.112884	-1.394786	-0.046381
39	9	0	-4.013898	-2.330234	0.323434
40	9	0	-3.666072	-0.709888	-1.070783
41	9	0	-2.057242	-2.078460	-0.579653
42	8	0	-1.021182	-1.211989	-3.457024
43	1	0	-1.598487	-1.491904	-2.735866
44	1	0	-0.600040	-0.391334	-3.094696

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.227941	-0.692006	-0.341903
2	6	0	0.782433	0.425108	0.294678
3	6	0	2.160851	0.586102	0.256139
4	6	0	3.012019	-0.316713	-0.403698
5	6	0	2.419992	-1.433106	-1.058712
6	6	0	1.039999	-1.599572	-1.041502
7	1	0	0.163712	1.135763	0.824791
8	6	0	4.447564	-0.098298	-0.414335
9	1	0	0.601497	-2.443944	-1.559996
10	6	0	4.896856	1.078515	0.296408
11	6	0	4.017133	1.906493	0.914194
12	1	0	5.956935	1.297205	0.331388
13	6	0	4.361873	3.144485	1.673074
14	1	0	5.439782	3.307956	1.671597
15	1	0	3.867326	4.013182	1.226136
16	1	0	4.013017	3.064132	2.707803
17	8	0	5.236260	-0.883217	-1.002623
18	8	0	3.198696	-2.315727	-1.713940
19	8	0	-0.233668	-2.656131	1.465600
20	8	0	2.677628	1.683417	0.902199
21	6	0	-1.253492	-3.065720	0.687074
22	1	0	-2.161508	-3.432975	1.228567
23	1	0	-1.009688	-3.915908	-0.002841
24	1	0	4.134365	-1.984222	-1.599846
25	6	0	-1.888866	-2.015682	-0.259053
26	8	0	-2.980066	-2.181873	-0.795182
27	7	0	-1.198094	-0.801248	-0.417620
28	6	0	-1.874956	0.258998	-1.116347
29	6	0	-2.825131	1.077466	-0.474587
30	6	0	-1.582373	0.485526	-2.463521
31	6	0	-3.470811	2.086006	-1.197080
32	6	0	-2.223945	1.498540	-3.174938
33	1	0	-0.844451	-0.144814	-2.948431
34	6	0	-3.176142	2.297111	-2.542894
35	1	0	-4.199729	2.712329	-0.697771
36	1	0	-1.984100	1.655791	-4.221817
37	1	0	-3.684426	3.084876	-3.088900
38	6	0	-3.138605	0.926183	0.992248
39	9	0	-2.027555	1.088604	1.769444
40	9	0	-4.031754	1.845788	1.416985
41	9	0	-3.646039	-0.283699	1.313440
42	8	0	-1.348043	-1.544990	3.513220
43	1	0	-1.684656	-0.725418	3.131655
44	1	0	-0.873777	-1.979903	2.716496

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.820869	-0.092050	0.136436
2	6	0	2.052369	0.519331	0.462238
3	6	0	3.234948	-0.078223	0.048880
4	6	0	3.273927	-1.279930	-0.676357
5	6	0	2.025899	-1.883703	-1.001182
6	6	0	0.831790	-1.297330	-0.604072
7	1	0	2.102366	1.444399	1.016384
8	6	0	4.542199	-1.862620	-1.072798
9	1	0	-0.097021	-1.783822	-0.870529
10	6	0	5.714737	-1.119464	-0.663685
11	6	0	5.604738	0.038831	0.033329
12	1	0	6.695091	-1.501584	-0.920257
13	6	0	6.736087	0.889722	0.506195
14	1	0	7.692359	0.449986	0.221870
15	1	0	6.661694	1.893700	0.075466
16	1	0	6.700783	0.996150	1.595332
17	8	0	4.612598	-2.950875	-1.703049
18	8	0	2.002946	-3.027640	-1.711503
19	8	0	-1.620944	-2.470008	3.154668
20	8	0	4.402406	0.562244	0.389682
21	6	0	-0.763384	-1.620551	2.388972
22	1	0	-0.146993	-2.262164	1.763956
23	1	0	-0.117665	-1.016935	3.036247
24	1	0	2.960871	-3.235788	-1.907828
25	6	0	-1.644932	-0.706392	1.548003
26	8	0	-2.511743	0.004720	2.020732
27	7	0	-0.437314	0.444086	0.496440
28	6	0	-0.441852	1.763840	1.065904
29	6	0	-0.611977	2.942236	0.295573
30	6	0	-0.257177	1.917907	2.447933
31	6	0	-0.579941	4.199182	0.914357
32	6	0	-0.238714	3.170536	3.056573
33	1	0	-0.111743	1.034392	3.055831
34	6	0	-0.396582	4.321175	2.288014
35	1	0	-0.379008	5.303045	2.749008
36	1	0	-2.287779	-1.892257	3.559610
37	6	0	-2.780958	-1.168979	-0.616262
38	8	0	-3.814686	-1.708305	-1.017609
39	8	0	-2.215245	-0.133257	-1.194500
40	8	0	-2.104432	-1.661056	0.440517
41	1	0	-1.392385	0.207067	-0.561997
42	19	0	-4.164950	0.271295	-3.079520
43	19	0	-3.426479	-3.902349	1.267663
44	1	0	-0.089275	3.242777	4.129393
45	1	0	-0.705333	5.086965	0.306957
46	6	0	-0.904878	2.934327	-1.184804

47	9	0	-0.184281	2.023379	-1.877340
48	9	0	-2.218628	2.670465	-1.432108
49	9	0	-0.652405	4.135247	-1.753913

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.184370	0.261432	-0.266982
2	6	0	2.437694	0.827406	0.044525
3	6	0	3.578051	0.073741	-0.187757
4	6	0	3.546353	-1.224060	-0.727683
5	6	0	2.270115	-1.770371	-1.049490
6	6	0	1.113902	-1.039662	-0.820814
7	1	0	2.532735	1.828302	0.442456
8	6	0	4.770729	-1.962286	-0.947866
9	1	0	0.149927	-1.468271	-1.067601
10	6	0	5.985511	-1.265747	-0.579007
11	6	0	5.946892	-0.010524	-0.068055
12	1	0	6.938345	-1.761113	-0.718937
13	6	0	7.125063	0.808225	0.343325
14	1	0	8.051594	0.257794	0.178082
15	1	0	7.156731	1.741585	-0.228353
16	1	0	7.051156	1.074407	1.402898
17	8	0	4.772140	-3.127268	-1.429518
18	8	0	2.193283	-3.009095	-1.571884
19	8	0	-0.477422	-0.916518	3.743553
20	8	0	4.779655	0.659215	0.130438
21	6	0	-0.761697	-1.868814	2.743604
22	1	0	-1.137977	-2.807450	3.176062
23	1	0	0.141066	-2.116149	2.169627
24	1	0	3.139106	-3.331291	-1.635418
25	6	0	-1.802340	-1.332563	1.776524
26	8	0	-2.335013	-0.249249	1.938741
27	7	0	-0.001707	0.948695	-0.093106
28	6	0	-0.184917	2.125526	0.658469
29	6	0	-0.975252	3.186254	0.160857
30	6	0	0.372075	2.253421	1.940626
31	6	0	-1.187821	4.329474	0.938421
32	6	0	0.171360	3.405141	2.696767
33	1	0	0.932078	1.421578	2.352540
34	6	0	-0.609962	4.449667	2.199342
35	1	0	-0.774707	5.345355	2.788497
36	1	0	-1.089665	-0.178185	3.579729
37	6	0	-2.833688	-1.616778	-0.393372
38	8	0	-3.919907	-2.177481	-0.553798
39	8	0	-2.236380	-0.742619	-1.032568
40	8	0	-2.055722	-2.168559	0.763081
41	1	0	-0.837031	0.492797	-0.462391
42	19	0	-4.283884	0.170167	-2.535499
43	19	0	-4.041210	-4.429856	0.941696
44	1	0	0.610155	3.475400	3.687251
45	1	0	-1.799546	5.131125	0.542416
46	6	0	-1.612512	3.103313	-1.198219
47	9	0	-0.737841	2.793671	-2.178833
48	9	0	-2.583246	2.135016	-1.237088
49	9	0	-2.217118	4.253888	-1.557022

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.135438	-0.940014	0.171385
2	6	0	-0.698608	0.340899	0.039494
3	6	0	-2.079591	0.458944	-0.017581
4	6	0	-2.944442	-0.644148	0.053189
5	6	0	-2.355240	-1.929062	0.193780
6	6	0	-0.973490	-2.070059	0.259117
7	1	0	-0.085792	1.226379	-0.033012
8	6	0	-4.383159	-0.459602	-0.013740
9	1	0	-0.557100	-3.060156	0.364577
10	6	0	-4.819550	0.911383	-0.162169
11	6	0	-3.926234	1.931091	-0.227435
12	1	0	-5.880246	1.121445	-0.222013
13	6	0	-4.258015	3.378157	-0.381540
14	1	0	-5.337493	3.521042	-0.435718
15	1	0	-3.862766	3.949844	0.464518
16	1	0	-3.797886	3.777463	-1.291355
17	8	0	-5.182173	-1.429354	0.052539
18	8	0	-3.142018	-3.020312	0.278309
19	8	0	3.662425	-1.164281	1.053174
20	8	0	-2.585500	1.730229	-0.155918
21	6	0	3.374491	-2.271707	0.324763
22	1	0	3.446695	-3.239125	0.879244
23	1	0	3.991984	-2.431433	-0.589233
24	1	0	-4.078821	-2.681150	0.215371
25	6	0	1.928032	-2.239021	-0.164899
26	8	0	1.400814	-3.127112	-0.826739
27	7	0	1.272161	-1.088925	0.270863
28	6	0	2.050554	0.018448	0.845756
29	6	0	2.497982	1.083655	-0.001935
30	6	0	1.749338	0.366558	2.194188
31	6	0	2.843301	2.324725	0.550017
32	6	0	2.087778	1.601853	2.713850
33	1	0	1.290802	-0.391770	2.821134
34	6	0	2.661396	2.596356	1.902216
35	1	0	3.239773	3.092323	-0.105739
36	1	0	1.887582	1.807982	3.762751
37	1	0	2.922068	3.567625	2.309380
38	6	0	2.655017	0.875274	-1.471085
39	9	0	1.471869	0.622206	-2.109527
40	9	0	3.185071	1.956671	-2.097319
41	9	0	3.458282	-0.176767	-1.797276

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.102130	-1.018119	0.278964
2	6	0	-0.640707	0.284853	0.259887
3	6	0	-2.012629	0.431415	0.121821
4	6	0	-2.898193	-0.651755	0.001115
5	6	0	-2.335731	-1.955186	0.026659
6	6	0	-0.964360	-2.132743	0.166757
7	1	0	-0.028649	1.169945	0.341815
8	6	0	-4.324551	-0.429774	-0.143637
9	1	0	-0.561970	-3.133660	0.172384
10	6	0	-4.731727	0.958382	-0.154861
11	6	0	-3.822002	1.958453	-0.034505
12	1	0	-5.782676	1.197078	-0.261553
13	6	0	-4.123402	3.420651	-0.033523
14	1	0	-5.195028	3.592535	-0.137590
15	1	0	-3.775856	3.878599	0.898327
16	1	0	-3.599762	3.916154	-0.857703
17	8	0	-5.140122	-1.382824	-0.251635
18	8	0	-3.140346	-3.032822	-0.080873
19	8	0	3.479907	-0.853226	1.100733
20	8	0	-2.493016	1.721993	0.102893
21	6	0	3.417244	-2.103288	0.456945
22	1	0	3.796220	-2.896516	1.113301
23	1	0	3.995043	-2.127640	-0.478925
24	1	0	-4.065250	-2.667863	-0.168271
25	6	0	1.957722	-2.355730	0.142087
26	8	0	1.527674	-3.415807	-0.310014
27	7	0	1.279714	-1.207072	0.439216
28	6	0	2.248485	-0.037385	0.887954
29	6	0	2.444196	1.018235	-0.137281
30	6	0	1.837270	0.517616	2.189705
31	6	0	2.213439	2.370193	0.144961
32	6	0	1.623938	1.854552	2.408463
33	1	0	1.719018	-0.207375	2.990593
34	6	0	1.777764	2.820768	1.385740
35	1	0	2.384432	3.086607	-0.653667
36	1	0	1.324938	2.173264	3.406332
37	1	0	1.600307	3.874466	1.571264
38	6	0	2.990063	0.648982	-1.458025
39	9	0	2.354902	-0.418838	-2.048739
40	9	0	2.929164	1.660102	-2.367215
41	9	0	4.315430	0.265395	-1.444860

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.168245	-1.022675	0.295169
2	6	0	-0.736657	0.267984	0.214909
3	6	0	-2.105205	0.382176	0.033372
4	6	0	-2.966253	-0.723967	-0.074842
5	6	0	-2.377673	-2.014867	0.009476
6	6	0	-1.008495	-2.159038	0.193006
7	1	0	-0.141643	1.166569	0.282332
8	6	0	-4.390130	-0.537418	-0.267609
9	1	0	-0.580263	-3.148939	0.238927
10	6	0	-4.826309	0.840989	-0.337015
11	6	0	-3.941778	1.863980	-0.225738
12	1	0	-5.878675	1.052495	-0.481025
13	6	0	-4.273770	3.318671	-0.282601
14	1	0	-5.345043	3.463461	-0.424921
15	1	0	-3.965385	3.814575	0.643645
16	1	0	-3.735373	3.798791	-1.106399
17	8	0	-5.185080	-1.509864	-0.367586
18	8	0	-3.159749	-3.111253	-0.087771
19	8	0	3.407642	-0.686593	1.245732
20	8	0	-2.612511	1.661430	-0.043983
21	6	0	3.368451	-1.963522	0.642126
22	1	0	3.760821	-2.707995	1.343867
23	1	0	3.970334	-2.006498	-0.276378
24	1	0	-4.088010	-2.766047	-0.213350
25	6	0	1.923315	-2.281742	0.305085
26	8	0	1.571479	-3.397274	-0.097524
27	7	0	1.201153	-1.156987	0.501011
28	6	0	2.268940	0.166317	0.969021
29	6	0	2.459131	1.132110	-0.115752

30	6	0	1.783389	0.769398	2.200404
31	6	0	2.041821	2.462611	0.011554
32	6	0	1.396612	2.087070	2.287247
33	1	0	1.732306	0.113746	3.064923
34	6	0	1.483953	2.962324	1.183762
35	1	0	2.181313	3.121880	-0.839717
36	1	0	1.027478	2.458990	3.241553
37	1	0	1.176416	3.999587	1.259498
38	6	0	3.126479	0.704222	-1.367637
39	9	0	2.563213	-0.406764	-1.945130
40	9	0	3.117332	1.662361	-2.331840
41	9	0	4.447097	0.362292	-1.209297

20-H$^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.722419	-0.989176	0.366409
2	6	0	-1.479563	0.186477	0.637119
3	6	0	-2.798750	0.269827	0.244774
4	6	0	-3.463350	-0.778484	-0.428645
5	6	0	-2.706356	-1.955467	-0.699127
6	6	0	-1.377262	-2.058402	-0.315074
7	1	0	-1.007028	1.014880	1.151391
8	6	0	-4.845170	-0.644641	-0.818902
9	1	0	-0.822476	-2.959370	-0.531375
10	6	0	-5.467414	0.618850	-0.471201
11	6	0	-4.775166	1.588308	0.176088
12	1	0	-6.504533	0.783635	-0.737046
13	6	0	-5.308224	2.922988	0.583566
14	1	0	-6.353376	3.026594	0.290066
15	1	0	-5.228119	3.049588	1.668369
16	1	0	-4.725474	3.724112	0.116736
17	8	0	-5.471731	-1.561354	-1.421892
18	8	0	-3.304035	-2.985941	-1.343109
19	8	0	3.180097	-0.537411	1.786848
20	8	0	-3.474338	1.439951	0.535125
21	6	0	2.843072	-1.791942	1.165489
22	1	0	2.968675	-2.515187	1.977087
23	1	0	3.561461	-2.057164	0.390064
24	1	0	-4.240603	-2.684063	-1.513920
25	6	0	1.423987	-1.978897	0.595528
26	8	0	1.269535	-3.091065	0.035131
27	7	0	0.580704	-0.964438	0.804112
28	6	0	3.067042	0.680135	1.186591
29	6	0	3.520647	1.047174	-0.102335
30	6	0	2.548181	1.685203	2.020207
31	6	0	3.389304	2.381739	-0.521461
32	6	0	2.441650	3.002493	1.595631
33	1	0	2.221401	1.387394	3.010520
34	6	0	2.852019	3.358198	0.307541
35	1	0	3.736016	2.649236	-1.512388
36	1	0	2.029304	3.750208	2.266675
37	1	0	2.766251	4.381776	-0.041214
38	6	0	4.176016	0.085649	-1.051945
39	9	0	3.301685	-0.792061	-1.613633
40	9	0	4.781860	0.717707	-2.083382
41	9	0	5.136414	-0.661301	-0.447282