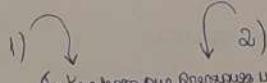


1) 
 Taken from our previous work (ref 17 from the
 SI pdf)

$$3) \begin{array}{r} 140 & 140 \\ 140 - 135 + 136 & 157 - 154 - 155 \\ \hline 140 & 140 \end{array}$$

$$4) \begin{array}{r} 140 & 140 \\ 140 - 135 + 136 & 157 - 154 - 155 \\ \hline 140 & 140 \end{array}$$

$$5) \begin{array}{r} 140 & 140 \\ 140 - 135 + 136 & 137 - 157 - 154 - 155 \\ \hline 135 & 140 \\ \hline 140 \end{array}$$

$$6) \begin{array}{r} 141 & 165 \\ 164 - 161 - 160 & - 162 - 163 \\ \hline 164 & 165 \end{array}$$

$$7) \begin{array}{r} 140 & 140 & 140 \\ 140 - 135 + 136 & 158 - 136 - 136 - 135 - 140 \\ \hline 140 & 154 \end{array}$$

$$8) \begin{array}{r} 140 & 140 & 140 \\ 140 - 135 + 136 & 137 - 157 - 154 - 155 \\ \hline 140 & 136 - 140 \\ \hline 140 \end{array}$$

$$9) \begin{array}{r} 965 \\ 965 - 961 + 962 & 961 - 965 \\ \hline 965 \end{array}$$

$$10) \begin{array}{r} 140 & 140 \\ 140 - 135 + 136 & 158 - 135 - 140 \\ \hline 140 & 154 \\ \hline 155 \end{array}$$

$$11) \begin{array}{r} 140 & 140 & 140 & 140 & 155 \\ 140 - 135 - 137 - 137 - 137 - 157 - 154 \\ \hline 135 & 135 & 135 \\ \hline 140 & 140 & 140 \\ \hline 140 \end{array}$$

$$12) \begin{array}{r} 140 & 140 \\ 140 - 135 - 136 + 137 & 158 - 154 - 155 \\ \hline 135 & 135 \\ \hline 140 & 140 \end{array}$$

$$13) \begin{array}{r} 140 \\ 140 - 135 - 159 - 154 - 155 \\ \hline 135 \\ \hline 140 \end{array}$$

$$14) \begin{array}{r} 140 & 140 \\ 135 - 136 & - 159 - 154 - 155 \\ \hline 140 \end{array}$$

15) $\begin{array}{c} 140_2 \\ | \\ 136 \\ | \\ 137-135 \\ | \\ 140_3 \end{array}$ 16) $\begin{array}{c} 40 \\ | \\ 140_2 \\ | \\ 136-137-136-153-154-155 \\ | \\ 140_2 \end{array}$
 $\begin{array}{c} 135-137 \\ | \\ 140_3 \\ | \\ 136 \\ | \\ 140_2 \\ | \\ 158 \\ | \\ 140 \\ | \\ 154 \\ | \\ 155 \end{array}$ $\begin{array}{c} 136 \\ | \\ 140_2 \\ | \\ 135 \end{array}$
 $\begin{array}{c} 140_2 \\ | \\ 136 \\ | \\ 136 \\ | \\ 140 \\ | \\ 140-137 \\ | \\ 137-135-140_3 \\ | \\ 135-158 \\ | \\ 140 \\ | \\ 154-155 \\ | \\ 140_3 \end{array}$

17) $\begin{array}{c} 140_2 \\ | \\ 136 \\ | \\ 136 \\ | \\ 140 \\ | \\ 140-137 \\ | \\ 137-135-140_3 \\ | \\ 135-158 \\ | \\ 140 \\ | \\ 154-155 \\ | \\ 140_3 \end{array}$ 18) $\begin{array}{c} 140_2 \\ | \\ 136-136 \\ | \\ 140_2 \\ | \\ 136 \\ | \\ 158 \\ | \\ 140 \\ | \\ 154-155 \\ | \\ 140 \end{array}$ 19) $\begin{array}{c} 140_2 \\ | \\ 136-136-136 \\ | \\ 140_2 \\ | \\ 136 \\ | \\ 140_2 \\ | \\ 136-140_2 \\ | \\ 140-158-136-136 \\ | \\ 154 \\ | \\ 140_2 \\ | \\ 155 \end{array}$
 $\begin{array}{c} 140_2 \\ | \\ 136 \\ | \\ 136 \\ | \\ 140 \\ | \\ 140-137 \\ | \\ 137-135-140_3 \\ | \\ 135-158 \\ | \\ 140 \\ | \\ 154-155 \\ | \\ 140_3 \end{array}$

* 20) $226-227 = 227-226$ 23) *Look from Sieganger.*
 21) $\begin{array}{c} 140_2 \\ | \\ 136 \\ | \\ 136 \\ | \\ 140_2 \\ | \\ 136 \\ | \\ 136-140_2 \\ | \\ 140_2 \\ | \\ 158 \\ | \\ 140 \\ | \\ 154-155 \\ | \\ 140 \end{array}$ 22) $\begin{array}{c} 153 \\ | \\ 153 \end{array}$ 25) $\begin{array}{c} 140_2 \\ | \\ 136-136 \\ | \\ 140_2 \\ | \\ 136-155 \\ | \\ 140-136 \\ | \\ 136-142 \\ | \\ 144 \\ | \\ 144 \end{array}$
 $\begin{array}{c} 140_2 \\ | \\ 136 \\ | \\ 136 \\ | \\ 140_2 \\ | \\ 136 \\ | \\ 136-140_2 \\ | \\ 140_2 \\ | \\ 158 \\ | \\ 140 \\ | \\ 154-155 \\ | \\ 140 \end{array}$ 24) $\begin{array}{c} 140_2 \\ | \\ 136-158-140 \\ | \\ 140_2 \\ | \\ 136-158-140 \\ | \\ 140_2 \\ | \\ 136-140_2 \\ | \\ 140-144 \\ | \\ 144 \end{array}$ 26) $324-268$
 $\begin{array}{c} 140_2 \\ | \\ 136 \\ | \\ 136 \\ | \\ 140_2 \\ | \\ 136 \\ | \\ 136-140_2 \\ | \\ 140_2 \\ | \\ 158 \\ | \\ 140 \\ | \\ 154-155 \\ | \\ 140 \end{array}$

* 27) $268-270$ 28) 120_3-135 30) $140-135$
 26) $324 = 142-144$ 27) $167-168$ 29) $140-135$
 $\begin{array}{c} 140_2 \\ | \\ 136 \\ | \\ 136 \\ | \\ 140_2 \\ | \\ 136 \\ | \\ 136-140_2 \\ | \\ 140_2 \\ | \\ 142 \\ | \\ 144 \\ | \\ 144 \end{array}$ $\begin{array}{c} 146 \\ | \\ 166-735 \\ | \\ 734-204 \\ | \\ 145 \\ | \\ 145 \\ | \\ 146-146 \\ | \\ 146 \end{array}$ $\begin{array}{c} 140 \\ | \\ 136 \\ | \\ 136 \\ | \\ 140_2 \\ | \\ 136 \\ | \\ 152-151 \\ | \\ 140 \\ | \\ 153 \end{array}$
 $\begin{array}{c} 140_2 \\ | \\ 136 \\ | \\ 136 \\ | \\ 140_2 \\ | \\ 136 \\ | \\ 136-140_2 \\ | \\ 140_2 \\ | \\ 142 \\ | \\ 144 \end{array}$

29) $140-135$ 31) $(170-169)-157-140_2$
 $\begin{array}{c} 140_2 \\ | \\ 136 \\ | \\ 136 \\ | \\ 140_2 \\ | \\ 136 \\ | \\ 140 \\ | \\ 906-911_2 \\ | \\ 900-903_2 \end{array}$ * part of the force field for having the come from Sieganger

32)

$$170 - 163 - 157 \left(\begin{array}{c} 140 \\ 136 \\ 140 \\ 140 \end{array} \right) 157 - 163 - 170$$

$$35) 140 - 135 \left(\begin{array}{c} 140 \\ 136 \\ 140 \\ 140 \end{array} \right) 957 - 956$$

34)

$$140 - 135 - 136 - 182 - 180 - 182 - 135 - 140 \left(\begin{array}{c} 140 \\ 185 \\ 140 \end{array} \right) 185$$

$$36) 140 - 135 \left(\begin{array}{c} 140 \\ 136 \\ 140 \\ 140 \end{array} \right) 957 - 722$$

37)

$$140 - 135 \left(\begin{array}{c} 140 \\ 136 \\ 140 \\ 140 \end{array} \right) 957$$

alarm type
taken from
Supergen
(which has the same
non-hardest parameter)

$$38) 140 - 135 \left(\begin{array}{c} 140 \\ 136 \\ 140 \end{array} \right) 136 - 277 = 278$$

$$40) 140 - 135 - 136 - 165 = 463$$

39)

$$140 - 135 - 136 - 280 - 136 - 135 - 140 \left(\begin{array}{c} 280 \\ 281 \\ 280 \\ 282 \\ 282 \end{array} \right)$$

$$\begin{array}{c} 140 \\ 135 \\ 140 \end{array}$$

41)

$$269 \left(\begin{array}{c} 140 \\ 267 \\ 268 \\ 140 \end{array} \right) 135 - 140$$

* part of the force
old parameterized force
from Supergen

42)

$$140 - 135 \left(\begin{array}{c} 140 \\ 136 \\ 140 \\ 759 \end{array} \right) 750 - 754 - 753$$

$$45) 202 = 212 = 202$$

46)

$$494 \left(\begin{array}{c} 493 \\ 494 \\ 493 - 494 \\ 140 \end{array} \right) 136 - 136$$

$$47) \begin{array}{c} 721 \\ 720 \\ 720 \\ 721 \\ 720 \\ 720 \\ 721 \end{array}$$

48) 800 from Supergen

$$49) \begin{array}{c} 170 \\ 170 - 171 - 173 - 174 - 173 \\ 171 \\ 170 \end{array}$$

50)

$$140 - 135 - 205 - 200 - 204 \left(\begin{array}{c} 140 \end{array} \right)$$

$$51) 140 - 135 - 136 - 152 - 151 \left(\begin{array}{c} 153 \\ 140 \\ 153 \end{array} \right)$$

140 140

52) $140_3 - 135 - 136 - 906 - 900 - 903 = 140_3$
 $140_2 \quad 906_2$

53) $140_3 - 135 - 180 - 180 - 180 - 135 - 140_3$
 $185_2 \quad 185_2$

54) $140_3 - 135 - 136 - 136 - 957 - 956 = 140_3$
 $140_2 \quad 140_2 \quad 958_2$

55) $140_3 - 135 - 136 - 136 - 136 - 135 - 140_3$
 $140_2 \quad 140_2 \quad 140_2$

56) $140_3 - 135 - 136 - 277 = 278$
 $140_2 \quad 277_2$

57) $140_3 - 136 - 267 = 269$
 $140_2 \quad 267_2$

58) $140_3 - 267 = 269$
 $140_2 \quad 269_2$

59) $279 - 267 = 263$
 $279_2 \quad 267_2$

60) $280_3 - 135 - 280 - 135 - 280_3 = 140_3$
 11_2
 281_2

61) $279 - 265 = 110_3$
 185_2

62) $279 - 235 = 236$
 234_2

*63) $759_3 - 755 - 754 = 753$
 754_2

*64) $144_3 - 143 = 517 - 154 - 155$
 185_2

*65) $958_3 - 957 - 956 = 958$
 154_2

*66) $155 - 154 - 154 = 753$

*67) $911_3 - 906_2 - 154 - 155$
 $900 - 909_2$

68) $140_3 - 206 - 200 - 204 = 140_3$
 $154 - 155_2$

70) $140_3 - 137 - 135 - 140_3$
 $140_2 \quad 136_2$

71) 140_3
 145_2
 $145_2 \quad 145_2 - 140_3$
 $145_2 \quad 145_2$
 146_2
 146_2

72) $280_3 - 135 - 280 - 136 - 135 - 140_3$
 $280_2 \quad 135_2$

73) 123
 $123 - 122 - 123$
 123

74) $264 - 263 = 146 - 145 - 140_3$
 $145 - 145_2$
 $145 - 145_2 \quad 145 - 140_3$
 146_2
 146_2

75) $140_3 - 136 - 136 - 136 - 140_3 = 140_3$
 $136 - 136_2$
 $140_2 \quad 140_2$

76) $140_3 - 136 - 136 - 136 - 400_2 = 140_3$
 $136 - 136_2$
 $140_2 \quad 140_2$

77) $151 - 150_2 - 150_2 - 151 = 153_2$
 $153_2 \quad 153_2$

* part of the force field parameters as the form digraphen

$$80) \quad 185 - 181 - 180$$

$$79) \quad 185_3 - 181_3 - 180_3 - 182_3 - 180_3 - 180_3 - 182_3 - 180_3 - 181_3 - 185_3 \\ 185_3 \quad 185_3 \quad 185_3 \quad 185_3$$

$$808) 170 - 169 - 157 - 157 - 169 - 170 \quad 81) 236 = 235 - 233 - 243 - 140_3 \quad 82) 440_3$$

$\begin{array}{r} 140 \\ 140 \end{array}$ $\begin{array}{r} 279 \\ 243 \\ -140_3 \end{array}$ $\begin{array}{r} 447 \\ 446 \end{array}$

$$83) \quad \begin{array}{r} 180 \\ 185 \\ -182 \\ \hline 182 \end{array} \quad \begin{array}{r} 180 \\ 185 \\ -180 \\ \hline 185 \end{array}$$

$$* 85) \quad 446 = 445 - 1$$

$\begin{array}{r} 902 + 905 - 911 \\ \swarrow \quad \searrow \\ 902 + 905 - 911 \end{array}$

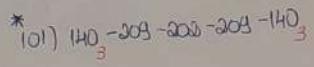
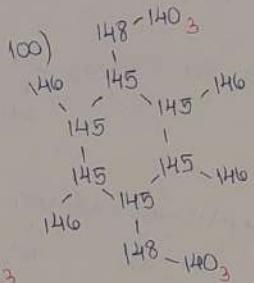
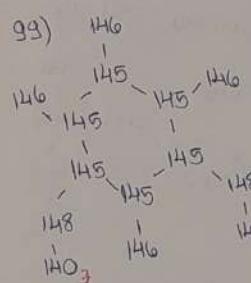
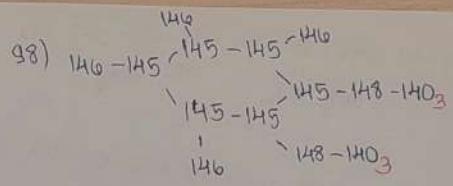
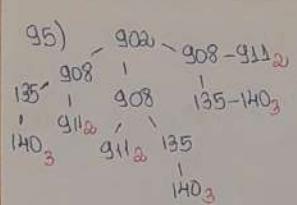
$\begin{array}{r} 902 + 905 - 911 \\ \swarrow \quad \searrow \\ 902 + 905 - 911 \end{array}$

$$87) \frac{140}{3} - 135 = 184 - 180 - 181 - 185_3 \quad * \quad 88) \frac{151}{3} - 152 - 153_2 = 911_3$$

$$90) \begin{array}{r} 140 \\ | \\ 140 \end{array} - 135 - 136 - 157 - 154 - 155$$

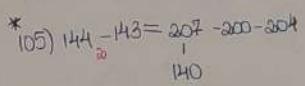
* part of the force field
parameters (some from
Sander)

* part of the force field parameters were from Siegert et al.



102) Daten from Supergen

103) Daten from Supergen



* part of the force field
parameters come from
Supergen.