Supporting Information

Prediction of thermodynamic properties of alkyne-containing mixtures with the *E*-PPR78 model

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Table S1. Group–interaction parameters: $(A_{kl} = A_{lk})$/MPa and $(B_{kl} = B_{lk})$/MPa. Only the parameters in the last three lines of this table, relative to groups 38, 39, 40 were determined in this work. The other parameters were determined in previous works [1-5].

	CH₃ (group 1)	CH₂ (group 2)	CH (group 3)	C (group 4)	CH₄ (group 5)	C₂H₆ (group 6)	CH_aro (group 7)	C_aro (group 8)	C_fused aromatic rings (group 9)	CH₂,cyclic (group 10)	CH_cyclic /C_cyclic (group 11)	CO₂ (group 12)	N₂ (group 13)
CH₃ (group 1)	0	-	-	-	-	-	-	-	-	-	-	-	-
CH₂ (group 2)	$A_{12}=65.54$ $B_{12}=105.7$	0	-	-	-	-	-	-	-	-	-	-	-
CH (group 3)	$A_{13}=214.9$ $B_{13}=294.9$	$A_{23}=39.05$ $B_{23}=41.59$	0	-	-	-	-	-	-	-	-	-	-
C (group 4)	$A_{14}=431.6$ $B_{14}=575.0$	$A_{24}=134.5$ $B_{24}=183.9$	$A_{34}=-86.13$ $B_{34}=85.10$	0	-	-	-	-	-	-	-	-	-
CH₄ (group 5)	$A_{15}=28.48$ $B_{15}=20.25$	$A_{25}=37.75$ $B_{25}=74.81$	$A_{35}=131.4$ $B_{35}=157.5$	$A_{45}=309.5$ $B_{45}=35.69$	0	-	-	-	-	-	-	-	-
C₂H₆ (group 6)	$A_{16}=3.775$ $B_{16}=8.922$	$A_{26}=29.85$ $B_{26}=65.88$	$A_{36}=156.1$ $B_{36}=96.77$	$A_{46}=388.1$ $B_{46}=-224.8$	$A_{56}=9.951$ $B_{56}=13.73$	0	-	-	-	-	-	-	-
CH_aro (group 7)	$A_{17}=98.83$ $B_{17}=136.2$	$A_{27}=25.05$ $B_{27}=64.51$	$A_{37}=56.62$ $B_{37}=129.7$	$A_{47}=170.5$ $B_{47}=284.1$	$A_{57}=67.26$ $B_{57}=167.5$	$A_{67}=41.18$ $B_{67}=50.79$	0	-	-	-	-	-	-
C_aro (group 8)	$A_{18}=103.60$ $B_{18}=103.60$	$A_{28}=5.147$ $B_{28}=-7.549$	$A_{38}=48.73$ $B_{38}=-89.22$	$A_{48}=128.3$ $B_{48}=189.1$	$A_{58}=106.7$ $B_{58}=190.8$	$A_{68}=67.94$ $B_{68}=210.7$	$A_{78}=-16.47$ $B_{78}=16.47$	0	-	-	-	-	-
C_fused aromatic rings (group 9)	$A_{19}=624.9$ $B_{19}=774.10$	$A_{29}=-17.84$ $B_{29}=-4.118$	NA	NA	$A_{59}=249.1$ $B_{59}=408.3$	NA	$A_{79}=52.50$ $B_{79}=251.2$	$A_{89}=-328.0$ $B_{89}=-569.3$	0	-	-	-	-
CH₂,cyclic (group 10)	$A_{1-10}=43.58$ $B_{1-10}=60.05$	$A_{2-10}=8.579$ $B_{2-10}=27.79$	$A_{3-10}=73.09$ $B_{3-10}=71.37$	$A_{4-10}=208.6$ $B_{4-10}=294.4$	$A_{5-10}=33.97$ $B_{5-10}=5.490$	$A_{6-10}=12.70$ $B_{6-10}=73.43$	$A_{7-10}=28.82$ $B_{7-10}=65.54$	$A_{8-10}=37.40$ $B_{8-10}=53.53$	$A_{9-10}=140.7$ $B_{9-10}=277.6$	0	-	-	-
CH_cyclic /C_cyclic (group 11)	$A_{1-11}=293.4$ $B_{1-11}=170.9$	$A_{2-11}=63.48$ $B_{2-11}=-74.46$	$A_{3-11}=-120.8$ $B_{3-11}=18.53$	$A_{4-11}=25.05$ $B_{4-11}=81.33$	$A_{5-11}=188.0$ $B_{5-11}=473.9$	$A_{6-11}=118.0$ $B_{6-11}=-212.8$	$A_{7-11}=129.0$ $B_{7-11}=36.72$	$A_{8-11}=-99.17$ $B_{8-11}=-193.5$	$A_{9-11}=-99.17$ $B_{9-11}=-193.5$	$A_{10-11}=139.0$ $B_{10-11}=35.69$	0	-	
CO₂ (group 12)	$A_{1-12}=144.8$ $B_{1-12}=401.5$	$A_{2-12}=141.4$ $B_{2-12}=237.1$	$A_{3-12}=191.8$ $B_{3-12}=380.9$	$A_{4-12}=377.5$ $B_{4-12}=162.7$	$A_{5-12}=136.6$ $B_{5-12}=214.8$	$A_{6-12}=136.2$ $B_{6-12}=235.7$	$A_{7-12}=98.48$ $B_{7-12}=253.6$	$A_{8-12}=154.4$ $B_{8-12}=374.4$	$A_{9-12}=331.1$ $B_{9-12}=276.6$	$A_{10-12}=144.1$ $B_{10-12}=354.1$	$A_{11-12}=216.2$ $B_{11-12}=-132.8$	0	
N₂ (group 13)	$A_{1-13}=38.09$ $B_{1-13}=88.19$	$A_{2-13}=83.73$ $B_{2-13}=188.7$	$A_{3-13}=383.6$ $B_{3-13}=375.4$	$A_{4-13}=341.8$ $B_{4-13}=635.2$	$A_{5-13}=30.88$ $B_{5-13}=37.06$	$A_{6-13}=61.59$ $B_{6-13}=84.92$	$A_{7-13}=185.3$ $B_{7-13}=490.7$	$A_{8-13}=343.8$ $B_{8-13}=1712$	$A_{9-13}=702.4$ $B_{9-13}=1889$	$A_{10-13}=179.5$ $B_{10-13}=546.6$	$A_{11-13}=331.5$ $B_{11-13}=389.8$	$A_{12-13}=113.9$ $B_{12-13}=212.4$	0

	CH$_3$ (group 1)	CH$_2$ (group 2)	CH (group 3)	C (group 4)	CH$_4$ (group 5)	C$_2$H$_6$ (group 6)	CH$_{aro}$ (group 7)	C$_{aro}$ (group 8)	C$_{fused aromatic rings}$ (group 9)	CH$_{2,cyclic}$ (group 10)	CH$_{cyclic}$/C$_{cyclic}$ (group 11)	CO$_2$ (group 12)	N$_2$ (group 13)
H$_2$S (group 14)	$A_{1-14}=159.6$ $B_{1-14}=227.8$	$A_{2-14}=136.6$ $B_{2-14}=124.6$	$A_{3-14}=192.5$ $B_{3-14}=562.8$	$A_{4-14}=330.8$ $B_{4-14}=-297.2$	$A_{5-14}=190.1$ $B_{5-14}=307.5$	$A_{6-14}=157.2$ $B_{6-14}=217.1$	$A_{7-14}=21.28$ $B_{7-14}=6.177$	$A_{8-14}=9.608$ $B_{8-14}=-36.72$	$A_{9-14}=9.608$ $B_{9-14}=-36.72$	$A_{10-14}=117.4$ $B_{10-14}=166.4$	$A_{11-14}=71.37$ $B_{11-14}=-127.7$	$A_{12-14}=135.2$ $B_{12-14}=199.0$	$A_{13-14}=319.5$ $B_{13-14}=550.1$
SH (group 15)	$A_{1-15}=789.6$ $B_{1-15}=1829$	$A_{2-15}=439.9$ $B_{2-15}=504.8$	$A_{3-15}=374.0$ $B_{3-15}=520.9$	$A_{4-15}=685.9$ $B_{4-15}=1547$	$A_{5-15}=701.7$ $B_{5-15}=1318$	NA	$A_{7-15}=277.6$ $B_{7-15}=449.5$	$A_{8-15}=1002$ $B_{8-15}=-736.4$	$A_{9-15}=1002$ $B_{9-15}=-736.4$	$A_{10-15}=493.1$ $B_{10-15}=832.1$	$A_{11-15}=463.2$ $B_{11-15}=-337.7$	NA	NA
H$_2$O (group 16)	$A_{1-16}=3557$ $B_{1-16}=11195$	$A_{2-16}=4324$ $B_{2-16}=12126$	$A_{3-16}=971.4$ $B_{3-16}=567.6$	NA	$A_{5-16}=2277.1$ $B_{5-16}=4719.6$	$A_{6-16}=2333$ $B_{6-16}=5147$	$A_{7-16}=2268$ $B_{7-16}=6218$	$A_{8-16}=543.5$ $B_{8-16}=411.8$	$A_{9-16}=1340$ $B_{9-16}=-65.88$	$A_{10-16}=4211$ $B_{10-16}=13031$	$A_{11-16}=244.0$ $B_{11-16}=-60.39$	$A_{12-16}=559.3$ $B_{12-16}=277.9$	$A_{13-16}=2574$ $B_{13-16}=5490$
C$_2$H$_4$ (group 17)	$A_{1-17}=7.892$ $B_{1-17}=35.00$	$A_{2-17}=59.71$ $B_{2-17}=82.35$	$A_{3-17}=147.9$ $B_{3-17}=-55.59$	$A_{4-17}=366.8$ $B_{4-17}=-219.3$	$A_{5-17}=19.22$ $B_{5-17}=33.29$	$A_{6-17}=7.549$ $B_{6-17}=20.93$	$A_{7-17}=25.74$ $B_{7-17}=78.92$	$A_{8-17}=97.80$ $B_{8-17}=67.94$	$A_{9-17}=209.7$ $B_{9-17}=3819$	$A_{10-17}=35.34$ $B_{10-17}=52.50$	$A_{11-17}=297.2$ $B_{11-17}=-647.2$	$A_{12-17}=73.09$ $B_{12-17}=106.7$	$A_{13-17}=45.30$ $B_{13-17}=92.65$
CH$_{2,alkenic}$/CH$_{alkenic}$ (group 18)	$A_{1-18}=48.73$ $B_{1-18}=44.27$	$A_{2-18}=9.608$ $B_{2-18}=50.79$	$A_{3-18}=84.76$ $B_{3-18}=193.2$	$A_{4-18}=181.2$ $B_{4-18}=419.0$	$A_{5-18}=48.73$ $B_{5-18}=68.29$	$A_{6-18}=26.77$ $B_{6-18}=-5.147$	$A_{7-18}=9.951$ $B_{7-18}=19.90$	$A_{8-18}=-48.38$ $B_{8-18}=27.79$	$A_{9-18}=669.8$ $B_{9-18}=589.5$	$A_{10-18}=-15.44$ $B_{10-18}=24.36$	$A_{11-18}=260.1$ $B_{11-18}=134.9$	$A_{12-18}=60.74$ $B_{12-18}=183.9$	$A_{13-18}=59.71$ $B_{13-18}=227.2$
C$_{alkenic}$ (group 19)	$A_{1-19}=102.6$ $B_{1-19}=260.1$	$A_{2-19}=64.85$ $B_{2-19}=51.82$	$A_{3-19}=91.62$ $B_{3-19}=54.90$	NA	NA	NA	$A_{7-19}=-16.47$ $B_{7-19}=61.42$	$A_{8-19}=343.1$ $B_{8-19}=880.2$	NA	$A_{10-19}=159.6$ $B_{10-19}=140.7$	NA	$A_{12-19}=74.81$ $B_{12-19}=-266.6$	$A_{13-19}=541.5$ $B_{13-19}=94.71$
CH$_{cycloalkenic}$/C$_{cycloalkenic}$ (group 20)	$A_{1-20}=47.01$ $B_{1-20}=169.5$	$A_{2-20}=34.31$ $B_{2-20}=51.13$	NA	NA	NA	NA	$A_{7-20}=3.775$ $B_{7-20}=1.716$	$A_{8-20}=242.9$ $B_{8-20}=-7.206$	NA	$A_{10-20}=31.91$ $B_{10-20}=69.32$	$A_{11-20}=151.3$ $B_{11-20}=2.745$	$A_{12-20}=87.85$ $B_{12-20}=66.91$	NA
H$_2$ (group 21)	$A_{1-21}=174.0$ $B_{1-21}=239.5$	$A_{2-21}=155.4$ $B_{2-21}=240.9$	$A_{3-21}=326.0$ $B_{3-21}=287.9$	$A_{4-21}=548.3$ $B_{4-21}=2343$	$A_{5-21}=156.1$ $B_{5-21}=92.99$	$A_{6-21}=137.6$ $B_{6-21}=150.0$	$A_{7-21}=288.9$ $B_{7-21}=189.1$	$A_{8-21}=400.1$ $B_{8-21}=1201$	$A_{9-21}=602.9$ $B_{9-21}=1463$	$A_{10-21}=236.1$ $B_{10-21}=192.5$	$A_{11-21}=-51.82$ $B_{11-21}=34.31$	$A_{12-21}=261.1$ $B_{12-21}=300.9$	$A_{13-21}=65.20$ $B_{13-21}=70.10$
C$_2$F$_6$ (group 22)	$A_{1-22}=119.1$ $B_{1-22}=118.4$	$A_{2-22}=105.0$ $B_{2-22}=130.4$	NA	NA	NA	$A_{6-22}=96.08$ $B_{6-22}=123.5$	NA	NA	NA	NA	NA	$A_{12-22}=126.6$ $B_{12-22}=241.2$	NA
CF$_3$ (group 23)	$A_{1-23}=123.2$ $B_{1-23}=133.8$	$A_{2-23}=195.6$ $B_{2-23}=199.0$	$A_{3-23}=531.5$ $B_{3-23}=-1945$	$A_{4-23}=413.1$ $B_{4-23}=975.2$	NA	$A_{6-23}=87.16$ $B_{6-23}=143.8$	$A_{7-23}=680.1$ $B_{7-23}=421.7$	$A_{8-23}=733.0$ $B_{8-23}=866.8$	NA	$A_{10-23}=216.2$ $B_{10-23}=343.1$	NA	$A_{12-23}=156.5$ $B_{12-23}=-116.0$	NA
CF$_2$ (group 24)	$A_{1-24}=58.33$ $B_{1-24}=65.20$	$A_{2-24}=58.33$ $B_{2-24}=68.63$	$A_{3-24}=-122.8$ $B_{3-24}=458.8$	$A_{4-24}=479.0$ $B_{4-24}=1430$	NA	$A_{6-24}=79.27$ $B_{6-24}=15.10$	$A_{7-24}=-31.57$ $B_{7-24}=43.24$	$A_{8-24}=-8.922$ $B_{8-24}=5.147$	NA	$A_{10-24}=42.55$ $B_{10-24}=-68.63$	NA	$A_{12-24}=125.2$ $B_{12-24}=340.1$	NA
CF$_{2,double bond}$ or CF$_{double bond}$ (group 25)	$A_{1-25}=-12.29$ $B_{1-25}=16.54$	NA	NA	NA	NA	$A_{6-25}=95.55$ $B_{6-25}=-231.1$	$A_{7-25}=-274.3$ $B_{7-25}=-411.7$	$A_{8-25}=78.62$ $B_{8-25}=-108.0$	NA	NA	NA	$A_{12-25}=36.25$ $B_{12-25}=63.49$	NA
C$_2$H$_4$F$_2$ (group 26)	$A_{1-26}=128.3$ $B_{1-26}=292.4$	$A_{2-26}=107.1$ $B_{2-26}=119.8$	$A_{3-26}=143.8$ $B_{3-26}=15.78$	NA	NA	NA	NA	NA	NA	NA	NA	$A_{12-26}=48.73$ $B_{12-26}=751.1$	NA
C$_2$H$_2$F$_4$ (group 27)	$A_{1-27}=158.5$ $B_{1-27}=356.5$	$A_{2-27}=86.47$ $B_{2-27}=-40.49$	$A_{3-27}=121.5$ $B_{3-27}=-44.61$	NA	NA	$A_{6-27}=72.40$ $B_{6-27}=-305.4$	NA	NA	NA	NA	NA	$A_{12-27}=29.51$ $B_{12-27}=89.90$	NA

	H_2S (group 14)	SH (group 15)	H_2O (group 16)	C_2H_4 (group 17)	$CH_{2,alkenic}$ /$CH_{alkenic}$ (group 18)	$C_{alkenic}$ (group 19)	$CH_{cycloalkenic}$ /$C_{cycloalkenic}$ (group 20)	H_2 (group 21)	C_2F_6 (group 22)	CF_3 (group 23)	CF_2 (group 24)	$CF_{2,double\ bond}$ or $CF_{double\ bond}$ (group 25)	$C_2H_4F_2$ (group 26)	$C_2H_2F_4$ (group 27)
H_2S (group 14)	0	-	-	-	-	-	-	-	-	-	-	-	-	-
SH (group 15)	$A_{14-15}=-157.8$ $B_{14-15}=153.7$	0	-	-	-	-	-	-	-	-	-	-	-	-
H_2O (group 16)	$A_{14-16}=603.9$ $B_{14-16}=599.1$	$A_{15-16}=30.88$ $B_{15-16}=-113.6$	0	-	-	-	-	-	-	-	-	-	-	-
C_2H_4 (group 17)	NA	NA	$A_{16-17}=1650$ $B_{16-17}=1661$	0	-	-	-	-	-	-	-	-	-	-
$CH_{2,alkenic}$ /$CH_{alkenic}$ (group 18)	NA	NA	$A_{16-18}=2243$ $B_{16-18}=5199$	$A_{17-18}=14.76$ $B_{17-18}=11.32$	0	-	-	-	-	-	-	-	-	-
$C_{alkenic}$ (group 19)	NA	NA	NA	$A_{17-19}=-518.2$ $B_{17-19}=6815$	$A_{18-19}=24.71$ $B_{18-19}=121.8$	0	-	-	-	-	-	-	-	-
$CH_{cycloalkenic}$ /$C_{cycloalkenic}$ (group 20)	NA	NA	NA	$A_{17-20}=-98.83$ $B_{17-20}=1809$	$A_{18-20}=14.07$ $B_{18-20}=-12.35$	$A_{19-20}=23.68$ $B_{19-20}=87.50$	0	-	-	-	-	-	-	-
H_2 (group 21)	$A_{14-21}=145.8$ $B_{14-21}=823.5$	NA	$A_{16-21}=830.8$ $B_{16-21}=-137.9$	$A_{17-21}=151.3$ $B_{17-21}=165.1$	$A_{18-21}=175.7$ $B_{18-21}=373.0$	$A_{19-21}=621.4$ $B_{19-21}=873.6$	$A_{20-21}=460.8$ $B_{20-21}=2167$	0	-	-	-	-	-	-
C_2F_6 (group 22)	NA	NA	NA	NA	$A_{18-22}=124.9$ $B_{18-22}=219.6$	NA	NA	NA	0	-	-	-	-	-
CF_3 (group 23)	NA	NA	NA	$A_{17-23}=453.0$ $B_{17-23}=-611.5$	$A_{18-23}=155.4$ $B_{18-23}=154.4$	NA	$A_{20-23}=1232$ $B_{20-23}=-495.5$	NA	$A_{22-23}=-14.47$ $B_{22-23}=-87.05$	0	-	-	-	-
CF_2 (group 24)	NA	NA	NA	NA	$A_{18-24}=155.4$ $B_{18-24}=154.4$	NA	NA	NA	NA	$A_{23-24}=0.000$ $B_{23-24}=0.000$	0	-	-	-
$CF_{2,double\ bond}$ or $CF_{double\ bond}$ (group 25)	NA	NA	NA	$A_{17-25}=-132.7$ $B_{17-25}=548.3$	$A_{18-25}=88.21$ $B_{18-25}=12.87$	NA	NA	NA	$A_{22-25}=55.90$ $B_{22-25}=-193.3$	$A_{23-25}=17.55$ $B_{23-25}=-92.99$	NA	0	-	-
$C_2H_4F_2$ (group 26)	NA	NA	NA	NA	$A_{18-26}=76.86$ $B_{18-26}=-145.5$	NA	NA	NA	NA	$A_{23-26}=113.2$ $B_{23-26}=247.1$	$A_{24-26}=120.1$ $B_{24-26}=264.2$	NA	0	-
$C_2H_2F_4$ (group 27)	NA	NA	NA	NA	$A_{18-27}=64.51$ $B_{18-27}=-41.86$	NA	NA	NA	$A_{22-27}=60.74$ $B_{22-27}=217.6$	$A_{23-27}=28.14$ $B_{23-27}=8.235$	$A_{24-27}=229.9$ $B_{24-27}=259.1$	NA	$A_{26-27}=-4.118$ $B_{26-27}=4.118$	0

	CH_3 (group 1)	CH_2 (group 2)	CH (group 3)	C (group 4)	CH_4 (group 5)	C_2H_6 (group 6)	CH_{aro} (group 7)	C_{aro} (group 8)	$C_{\text{fused aromatic rings}}$ (group 9)	$CH_{2,cyclic}$ (group 10)	CH_{cyclic}/C_{cyclic} (group 11)	CO_2 (group 12)	N_2 (group 13)
CO (group 28)	$A_{1-28}=91.24$ $B_{1-28}=94.24$	$A_{2-28}=44.00$ $B_{2-28}=45.55$	NA	NA	$A_{5-28}=14.43$ $B_{5-28}=20.92$	$A_{6-28}=15.42$ $B_{6-28}=33.30$	$A_{7-28}=153.4$ $B_{7-28}=153.4$	$A_{8-28}=125.77$ $B_{8-28}=-231.1$	$A_{9-28}=197.0$ $B_{9-28}=-238.8$	$A_{10-28}=113.1$ $B_{10-28}=143.6$	NA	$A_{12-28}=87.85$ $B_{12-28}=190.8$	$A_{13-28}=23.33$ $B_{13-28}=-25.40$
He (group 29)	$A_{1-29}=416.3$ $B_{1-29}=513.4$	$A_{2-29}=520.52$ $B_{2-29}=673.22$	$A_{3-29}=728.1$ $B_{3-29}=750.9$	NA	$A_{5-29}=394.5$ $B_{5-29}=378.1$	$A_{6-29}=581.3$ $B_{6-29}=517.1$	$A_{7-29}=753.6$ $B_{7-29}=590.5$	$A_{8-29}=753.6$ $B_{8-29}=590.5$	$A_{9-29}=753.6$ $B_{9-29}=590.5$	NA	NA	$A_{12-29}=685.9$ $B_{12-29}=559.3$	$A_{13-29}=204.7$ $B_{13-29}=222.8$
Ar (group 30)	$A_{1-30}=11.27$ $B_{1-30}=55.48$	$A_{2-30}=113.6$ $B_{2-30}=231.6$	$A_{3-30}=185.8$ $B_{3-30}=634.2$	$A_{4-30}=899.0$ $B_{4-30}=4655$	$A_{5-30}=15.97$ $B_{5-30}=24.48$	$A_{6-30}=43.81$ $B_{6-30}=53.10$	$A_{7-30}=195.6$ $B_{7-30}=361.3$	NA	NA	$A_{10-30}=1269$ $B_{10-30}=18666$	NA	$A_{12-30}=177.8$ $B_{12-30}=86.82$	$A_{13-30}=6.488$ $B_{13-30}=8.774$
SO_2 (group 31)	$A_{1-31}=322.2$ $B_{1-31}=201.4$	$A_{2-31}=55.9$ $B_{2-31}=-28.5$	$A_{3-31}=-70.0$ $B_{3-31}=233.7$	NA	$A_{5-31}=205.9$ $B_{5-31}=323.6$	NA	$A_{7-31}=37.1$ $B_{7-31}=-23.7$	$A_{8-31}=-196.6$ $B_{8-31}=-397.4$	NA	NA	NA	$A_{12-31}=54.90$ $B_{12-31}=59.02$	$A_{13-31}=282.4$ $B_{13-31}=362.7$
O_2 (group 32)	$A_{1-32}=86.1$ $B_{1-32}=87.5$	$A_{2-32}=107.4$ $B_{2-32}=200.8$	NA	NA	NA	NA	$A_{7-32}=233.4$ $B_{7-32}=404.9$	$A_{8-32}=177.1$ $B_{8-32}=2559.4$	NA	$A_{10-32}=181.2$ $B_{10-32}=281.4$	$A_{11-32}=102.3$ $B_{11-32}=988.0$	$A_{12-32}=154.4$ $B_{12-32}=109.8$	$A_{13-32}=2.40$ $B_{13-32}=4.80$
NO (group 33)	NA	NA	NA	NA	NA	NA	NA	NA	NA	$A_{10-33}=-27.5$ $B_{10-33}=50.1$	NA	$A_{12-33}=5.1$ $B_{12-33}=48.4$	$A_{13-33}=258.7$ $B_{13-33}=100.5$
COS (group 34)	NA	NA	NA	NA	$A_{5-34}=44.61$ $B_{5-34}=-95.05$	NA	NA	NA	NA	NA	NA	$A_{12-34}=83.04$ $B_{12-34}=165.7$	NA
NH_3 (group 35)	NA	NA	NA	NA	$A_{5-35}=436.1$ $B_{5-35}=958.8$	NA	NA	NA	NA	NA	NA	NA	$A_{13-35}=585.8$ $B_{13-35}=1011.3$
NO_2/N_2O_4 (group 36)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	$A_{12-36}=124.9$ $B_{12-36}=241.6$	$A_{13-36}=263.5$ $B_{13-36}=260.0$
N_2O (group 37)	NA	NA	NA	NA	$A_{5-37}=74.81$ $B_{5-37}=107.1$	NA	NA	NA	NA	NA	NA	$A_{12-37}=3.77$ $B_{12-37}=14.07$	$A_{13-37}=101.6$ $B_{13-37}=230.9$
C_2H_2 (group 38)	$A_{1-38}=-6.86$ $B_{1-38}=41.52$	$A_{2-38}=421.0$ $B_{2-38}=1193.8$	NA	NA	NA	$A_{6-38}=137.9$ $B_{6-38}=168.1$	$A_{7-38}=29.17$ $B_{7-38}=123.5$	NA	NA	NA	NA	NA	NA
HC≡C- (group 39)	$A_{1-39}=306.1$ $B_{1-39}=1167.0$	$A_{2-39}=303.3$ $B_{2-39}=316.0$	$A_{3-39}=206.9$ $B_{3-39}=3975.0$	NA	NA	NA	$A_{7-39}=96.08$ $B_{7-39}=148.2$	$A_{8-39}=176.0$ $B_{8-39}=-459.5$	NA	$A_{10-39}=496.2$ $B_{10-39}=496.2$	$A_{11-39}=863.7$ $B_{11-39}=863.7$	$A_{12-39}=60.05$ $B_{12-39}=-80.98$	NA
-C≡C- (group 40)	$A_{1-40}=72.06$ $B_{1-40}=1219.5$	$A_{2-40}=488.0$ $B_{2-40}=826.6$	$A_{3-40}=4.46$ $B_{3-40}=-245.4$	NA	NA	NA	$A_{7-40}=403.9$ $B_{7-40}=403.9$	$A_{8-40}=518.5$ $B_{8-40}=518.5$	NA	$A_{10-40}=845.9$ $B_{10-40}=845.9$	NA	NA	NA

	H$_2$S (group 14)	SH (group 15)	H$_2$O (group 16)	C$_2$H$_4$ (group 17)	CH$_{2,alkenic}$/CH$_{alkenic}$ (group 18)	C$_{alkenic}$ (group 19)	CH$_{cycloalkenic}$/C$_{cycloalkenic}$ (group 20)	H$_2$ (group 21)	C$_2$F$_6$ (group 22)	CF$_3$ (group 23)	CF$_2$ (group 24)	CF$_{2,double bond}$ or CF$_{double bond}$ (group 25)	CHF$_2$-CH$_3$ (group 26)	CF$_3$-CH$_2$F (group 27)
CO (group 28)	A$_{14-28}$ = 278.6 B$_{14-28}$ = 404.2	NA	A$_{16-28}$ = 715.1 B$_{16-28}$ = −89.90	A$_{17-28}$ = 84.55 B$_{17-28}$ = −7.515	NA	NA	NA	A$_{21-28}$ = 75.84 B$_{21-28}$ = 74.81	NA	NA	NA	NA	NA	NA
He (group 29)	NA	NA	NA	A$_{17-29}$ = 569.6 B$_{17-29}$ = 536.7	A$_{18-29}$ = 644.3 B$_{18-29}$ = 687.7	NA	NA	A$_{21-29}$ = 138.7 B$_{21-29}$ = 95.49	NA	NA	NA	NA	NA	NA
Ar (group 30)	NA	NA	A$_{16-30}$ = 1197 B$_{16-30}$ = 1211	NA	A$_{18-30}$ = 203.0 B$_{18-30}$ = −11.78	NA	NA	A$_{21-30}$ = 128.2 B$_{21-30}$ = 102.9	NA	NA	NA	NA	NA	NA
SO$_2$ (group 31)	NA	NA	A$_{16-31}$ = 374.4 B$_{16-31}$ = 148.6	NA	A$_{18-31}$ = 26.8 B$_{18-31}$ = 26.8	A$_{19-31}$ = −141.7 B$_{19-31}$ = −151.3	NA	NA	NA	NA	NA	NA	NA	NA
O$_2$ (group 32)	NA	NA	A$_{16-32}$ = 1376 B$_{16-32}$ = 1609	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
NO (group 33)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
COS (group 34)	A$_{14-34}$ = 101.9 B$_{14-34}$ = 98.14	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
NH$_3$ (group 35)	NA	NA	A$_{16-35}$ = −550.1 B$_{16-35}$ = −1404.2	NA	NA	NA	NA	A$_{21-35}$ = 701.7 B$_{21-35}$ = 931.3	NA	NA	NA	NA	NA	NA
NO$_2$/N$_2$O$_4$ (group 36)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
N$_2$O (group 37)	NA	NA	A$_{16-37}$ = 568.9 B$_{16-37}$ = −144.8	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
C$_2$H$_2$ (group 38)	NA	NA	A$_{16-38}$ = 436.8 B$_{16-38}$ = −200.1	NA	A$_{18-38}$ = 165.4 B$_{18-38}$ = 39.80	NA	NA	NA	NA	NA	NA	NA	A$_{26-38}$ = −58.68 B$_{26-38}$ = 303.7	NA
HC≡C- (group 39)	NA	NA	A$_{16-39}$ = −2395.5 B$_{16-39}$ = −11671	NA	A$_{18-39}$ = 134.5 B$_{18-39}$ = 568.9	A$_{19-39}$ = 212.8 B$_{19-39}$ = −2182.8	NA	NA	NA	NA	NA	NA	NA	NA
-C≡C- (group 40)	NA	NA	NA	NA	A$_{18-40}$ = 255.6 B$_{18-40}$ = 676.7	A$_{19-40}$ = −874.3 B$_{19-40}$ = 1040.1	NA	NA	NA	NA	NA	NA	NA	NA

	CO (group 28)	He (group 29)	Ar (group 30)	SO₂ (group 31)	O₂ (group 32)	NO (group 33)	COS (group 34)	NH₃ (group 35)	NO₂/N₂O₄ (group 36)	N₂O (group 37)	C₂H₂ (group 38)	HC≡C- (group 39)	-C≡C- (group 40)
CO (group 28)	0	-	-										
He (group 29)	$A_{28-29}=260.1$ $B_{28-29}=259.9$	0	-										
Ar (group 30)	$A_{28-30}=4.042$ $B_{28-30}=8.180$	$A_{29-30}=243.1$ $B_{29-30}=305.6$	0										
SO₂ (group 31)	**NA**	**NA**	$A_{30-31}=299.9$ $B_{30-31}=354.1$	0									
O₂ (group 32)	**NA**	**NA**	$A_{30-32}=4.80$ $B_{30-32}=7.89$	$A_{31-32}=340.0$ $B_{31-32}=665.7$	0								
NO (group 33)	$A_{28-33}=309.2$ $B_{28-33}=28.82$	**NA**	$A_{30-33}=110.8$ $B_{30-33}=155.5$	$A_{31-33}=172.3$ $B_{31-33}=1343$	**NA**	0							
COS (group 34)	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	0						
NH₃ (group 35)	**NA**	**NA**	$A_{30-35}=630.0$ $B_{30-35}=1794.0$	**NA**	**NA**	**NA**	**NA**	0					
NO₂/N₂O₄ (group 36)	**NA**	**NA**	$A_{30-36}=278.6$ $B_{30-36}=274.5$	**NA**	$A_{32-36}=271.1$ $B_{32-36}=362.4$	**NA**	**NA**	**NA**	0				
N₂O (group 37)	**NA**	**NA**	**NA**	**NA**	$A_{32-37}=120.1$ $B_{32-37}=105.7$	**NA**	**NA**	**NA**	**NA**	0			
C₂H₂ (group 38)	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	0		
HC≡C- (group 39)	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	$A_{38-39}=122.5$ $B_{38-39}=247.8$	0	
-C≡C- (group 40)	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	$A_{39-40}=-497.6$ $B_{39-40}=-824.2$	0

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