Pot a00_1 : Initial calculations – See plot for the values of the atom-atom parameters quadrupole moment in 10^-26 esu = 2.0100 2.0100 -4.0200 vibrational dependence of polarizability : 0.263900E+010.100000E+000.516000E-010.223600E+00



Pot a00_2 : Pot a00_1 with a reduction of 5% of the quadrupole moment of CO_2 quadrupole moment in 10^-26 esu = 1.9100 1.9100 -3.8200 vibrational dependence of polarizability 0.263900E+010.100000E+000.516000E-010.223600E+00





Pot a25_1 : (From Pot a00_1) Increase of 60% of ε (ON), Reduction of 2.6% of σ (ON), Reduction of 72% of ε (traj), Reduction of 17% of σ (traj)

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quadrupole moment in 10⁻²⁶ esu = 1.8900 1.8900 -3.7800 vibrational dependence of polarizability 0.263900E+010.120000E+000.618000E-010.268000E+00



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Pot a25_2 : Pot a25_1 with a reduction of 2.2% of quadrupole moment of CO₂ (or 8% from Pot a00_1), and increase of 33% of polarizability coefficients

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Pot a25_3 : Pot a25_1 with a reduction of 2.2% of quadrupole moment of CO₂ (or 8% from Pot a00_1), and increase of 20% of polarizability coefficients

quadrupole moment in 10⁻²⁶ esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.150000E+000.750000E-010.268000E+00

N₂ measurement vs. esiculation 30012 00001 e1;c2;c3= 0.15 0.08 0.27



Pot a25_4 : Pot a25_1 with a reduction of 2.2% of the quadrupole moment of CO_2 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.120000E+000.600000E-010.268000E+00



Pot a26_1 : (From Pot a00_1) Increase of 60% of ε(ON), Increase of 2.5% of σ(ON), Reduction of 72% of ε(traj), Reduction of 17% of $\sigma(\text{traj})$

quadrupole moment in 10^{-26} esu = 1.8490 1.8490 -3.6980vibrational dependence of polarizability 0.263900E+010.160000E+000.810000E-010.268000E+00



m

Pot a26_2 : Pot a26_1 with a reduction of 14.5% of the polarizability coefficients quadrupole moment in 10^{-26} esu = 1.8490 1.8490 -3.6980vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00



Pot a27_1 : (From Pot a00_1) Increase of 60% of ε (ON), Reduction of 2.6% of σ (ON), Reduction of 72% of ε (traj), Reduction of 11% of σ (traj)

quadrupole moment in 10⁻²⁶ esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.160000E+000.810000E-010.268000E+00



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-50

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-30

-20

-10

n.

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Pot a27_2 : Pot a27_1 with a reduction of 14.3% of the polarizability coefficients



Pot a28 : (From Pot a00_1) Increase of 60% of ε(ON), Reduction of 2.6% of σ(ON), Reduction of 64% of ε(traj), Reduction of 16.7% of σ(traj)



quadrupole moment in 10^{-26} esu = 1.8490 1.8490 -3.6980

Pot a29_1 : (From Pot a00_1) Increase of 60% of ε (ON), Reduction of 2.6% of σ (ON), Reduction of 32.6% of ε (traj), Reduction of 16.7% of σ (traj)

quadrupole moment in 10⁻²⁶ esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.160000E+000.810000E-010.268000E+00



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Pot a29_2 : Pot a29_1 with a reduction of 14.3% of the polarizability coefficients quadrupole moment in 10^{-26} esu = 1.8490 1.8490 -3.6980vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00



Pot a30 : (From Pot a00_1) Increase of 96.6% of ε (ON), Reduction of 2.6% of σ (ON), Reduction of 32.6% of ε (traj), Reduction of 11% of σ (traj)

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quadrupole moment in 10⁻²⁶ esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.160000E+000.810000E-010.268000E+00



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Pot a31 1 : (From Pot a00 1) Increase of 96.6% of ε (ON), Reduction of 2.6% of σ (ON), Reduction of 72% of ε (traj), Reduction of 11% of $\sigma(traj)$

quadrupole moment in 10^{-26} esu = 1.8490 1.8490 -3.6980vibrational dependence of polarizability 0.263900E+010.160000E+000.810000E-010.268000E+00



m

Pot a31_2 : Pot a31_1 with a reduction of 14.3% of the polarizability coefficients



Pot a32 : (From Pot a00 1) Increase of 57.3% of ε (ON), Reduction of 2.6% of σ (ON), Reduction of 32.6% of ε (traj), Reduction of 6.1% of $\sigma(traj)$

quadrupole moment in 10^{-26} esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.160000E+000.810000E-010.268000E+00

4 4







Pot a33 : (From Pot a00_1) Increase of 57.3% of ε (ON), Reduction of 2.6% of σ (ON), Reduction of 32.6% of ε (traj), Reduction of 1.5% of σ (traj)

quadrupole moment in 10^{-26} esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.160000E+000.810000E-010.268000E+00



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Pot a34 : (From Pot a00_1) Increase of 216% of ε(ON), Reduction of 2.6% of σ(ON), Reduction of 20.6% of ε(traj), Reduction of 1.1% of $\sigma(\text{traj})$

00001 e1.c2.c3+ 0.18 0.08 0.27 $Ord_L1m_L2m = 20$ 4 4 🛦 Devî et al. €/k (K) 94.94 51.28 = 3.07 3.42 - (**8**1 111.41624 3.9847 =12-6Έġ. % Difference= -14.14 SD= 1.89 N= 51 CO2-N2 line shifts 30012 00001 atm⁻¹ -5x % Difference= -9.39 SD= 12.97 N= 51 -60 -70-60 -50 -40 -30 -2010 20 30 40 50 60 70 80 0 m CO₂-N₂ temp dep 30012 00001 ▲ Predoi-Cross et al. A Gamache -80 -70 -60 -50 -40 -30 -20-10 n 10 20 -30 40 50 60 70 80 m

Pot a35 : (From Pot a00_1) Increase of 49% of ε (ON), Reduction of 2.6% of σ (ON), Reduction of 13.7% of ε (traj), Reduction of 11% of σ (traj)

quadrupole moment in 10⁻²⁶ esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.160000E+000.810000E-010.268000E+00

00₂-N₂ (

esumement vs. esiculation 30012 00001 e1,c2,c3= 0.18 0.08 0.27



Pot a38 : (From Pot a00_1) Increase of 57.3% of ε(ON), Increase of 2.3% of σ(ON), Reduction of 32.6% of ε(traj), Reduction of 22.9% of $\sigma(traj)$

quadrupole moment in 10^{-26} esu = 1.8490 1.8490 -3.6980vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00



m

Pot a39 : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 2.5% of σ (ON), Reduction of 32.6% of ε (traj), Reduction of 22.9% of σ (traj)

quadrupole moment in 10⁻²⁶ esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00



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Pot a40 : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 2.5% of σ (ON), Reduction of 32.6% of ε (traj), Reduction of 29.3% of σ (traj)



Pot a42 : (From Pot a00_1) Increase of 18% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 32.6% of ε (traj), Reduction of 22.9% of σ (traj)

 quadrupole moment in 10^{-26} esu = 1.8490
 1.8490
 -3.6980

 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00

 (0, -1), measurement is, celectation



Pot a43 : (From Pot a00_1) Increase of 18% of ε(ON), Increase of 7.3% of σ(ON), Reduction of 32.6% of ε(traj), Reduction of 20.2% of $\sigma(\text{traj})$



quadrupole moment in 10^{-26} esu = 1.8490 1.8490 -3.6980

Pot a44 : (From Pot a00_1) Increase of 18% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 32.6% of ε (traj), Reduction of 29.3% of σ (traj)

00,-N, I 00001 e1 c2 c3= 0.14 0.07 0.23 Ord,L1m,L2m = 20 4 4 🛓 Devî et al. €/k (K) 51.79 51.28 = σ (Å) 3.38 3.42 3.1136 Ĩ, 101.28749 18 ш =12-6Ti = 75.0 K % Difference= 0.72 SD= 1.46 N= 51 CO₂-N₂ line shifts 30012 00001 ð / em⁻¹ atm⁻¹ -0.01 -5×10⁻ %, Difference=, -11.65 \$D=, 12.22 N=, 51 -60 -70 -60 -40 -30 10 20 40 50 60 70 80 -20 30012 00001 CO₂-N₂ temp dep ▲ Predoi-Cross et al. 🛓 Gamache c -50 -30 -20 -10 0 10 20 -40

Pot a45 : (From Pot a00_1) Increase of 0.3% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 32.6% of ε (traj), Reduction of 20.2% of σ (traj)

00,-N, I 00001 e1 c2 c3= _0.14 (0.07 (0.23 Ord,L1m,L2m = 20 4 4 🛓 Devî et al. 44.02 51.28 €/k (K) = σ (Å) 3.38 3.42 ours atm¹¹ 3.3500 101.28749 ш =12-6Ti = 75.0 K -0.63 SD= 2.02 N= 5 % Difference= CO₂-N₂ line shifts 30012 00001 ð / cm⁻¹ atm⁻¹ -0.01 -5×10⁻¹ % Difference= -10.66 SD= 13.13 N= 51 -60 -70 -60 -40 -30 10 20 40 50 60 70 80 -20 30012 00001 CO₂-N₂ temp dep ▲ Predoi-Cross et al. 🛓 Gamache c 12-Sep--50 -40 -30 -20 -10 0 10 20 .30 50 60 80 -80

Pot a46 : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 2.5% of σ (ON), Reduction of 39.6% of ε (traj), Reduction of 20.2% of σ (traj)

^{00&}lt;sub>2</sub>-N₂ measurement vs. colculation 30012 00001 c1,c2,c3= 0.14 0.07 0.27



Pot a47 : (From Pot a00_1) Increase of 8.5% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 32.6% of ε (traj), Reduction of 20.2% of σ (traj)



Pot a48 : (From Pot a00_1) Increase of 8.5% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 32.6% of ε (traj), Reduction of 39.6% of σ (traj)

00,-N, I 00001 e1 c2 c3= 0.14 0.07 0.23 $0nd_{L1m_{L2m}} = 20$ 4 4 🛓 Devî et al. €/k (K) 47.64 51.28 = σ (Å) 3.38 3.42 am⁻¹ atm⁻¹ 0.05 3.3500 96.22312 1.1 =12-6Ti = 75.0 K -0.98 SD= 1.62 N= 51 % Difference= CO₂-N₂ line shifts 30012 00001 ð / cm⁻¹ atm⁻¹ -0.01 -5×10⁻ % Difference= -10.79 SD= 12.50 N= 51 -60 -70 -60 -40 -30 10 20 40 50 60 70 80 -20 30012 00001 CO₂-N₂ temp dep ▲ Predoi-Cross et al. 🛓 Gamache c 12-Sep -50 -40 -30 -20 -10 0 10 20 50 60 80

Pot a55 : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 32.6% of ε (traj), Reduction of 21.4% of σ (traj)

 ϵ (ON)= 58.69 ; σ (ON)=3.23 ; ϵ (traj)= 101.28749 ; σ (traj)=3.31650 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00



Pot a56 : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 32.6% of ε (traj), Reduction of 21.1% of σ (traj)

 ϵ (ON)= 58.69 ; σ (ON)=3.23 ; ϵ (traj)= 101.28749 ; σ (traj)=3.32655 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00



Pot a57 : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 39.6% of ε (traj), Reduction of 20.2% of σ (traj)

 ϵ (ON)= 58.69 ; σ (ON)=3.23 ; ϵ (traj)= 96.22312 ; σ (traj)=3.35000 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00



Pot a58 : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 31.3% of ε (traj), Reduction of 22.9% of σ (traj)

 ϵ (ON)= 58.69 ; σ (ON)=3.23 ; ϵ (traj)= 102.30036 ; σ (traj)= 3.27750 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00



Pot a59 : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 31% of ε (traj), Reduction of 22.9% of σ (traj)

 ϵ (ON)= 58.69 ; σ (ON)=3.23 ; ϵ (traj)= 102.50294 ; σ (traj)= 3.27750 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00



Pot a60 : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 30.7% of ε (traj), Reduction of 22.9% of σ (traj)

 ϵ (ON)= 58.69 ; σ (ON)=3.23 ; ϵ (traj)= 102.80680 ; σ (traj)= 3.27750 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00



Pot a61 : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 30.8% of ε (traj), Reduction of 22.9% of σ (traj)

 ϵ (ON)= 58.69 ; σ (ON)=3.23 ; ϵ (traj)= 102.65487 ; σ (traj)= 3.27750 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00



Pot a62 : (From Pot a00_1) Increase of 18% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 32.6% of ε (traj), Reduction of 20.2% of σ (traj)

 ϵ (ON)= 51.79 ; σ (ON)=3.23 ; ϵ (traj)= 101.28749 ; σ (traj)= 3.35000 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00



Pot a63 : (From Pot a00_1) Increase of 33.9% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 39.6% of ε (traj), Reduction of 22.9% of σ (traj)

 ϵ (ON)= 58.79 ; σ (ON)=3.23 ; ϵ (traj)= 96.22311 ; σ (traj)= 3.27750 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00



Pot a64 : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 20.6% of ε (traj), Reduction of 22.9% of σ (traj)

 ϵ (ON)= 58.69 ; σ (ON)=3.23 ; ϵ (traj)= 111.41624 ; σ (traj)= 3.27750 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00

Pot a65 : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 9.5% of ε (traj), Reduction of 25.6% of σ (traj)

 ϵ (ON)= 58.69 ; σ (ON)=3.23 ; ϵ (traj)= 122.55786 ; σ (traj)= 3.20657 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00

Pot a66 : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 7.3% of σ (ON), Increase of 0.4% of ε (traj), Reduction of 28.4% of σ (traj)

 ϵ (ON)= 58.69 ; σ (ON)=3.23 ; ϵ (traj)= 134.81365 ; σ (traj)= 3.13717 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00

Pot a67 : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 24.8% of ε (traj), Reduction of 22.9% of σ (traj)

 ϵ (ON)= 58.69 ; σ (ON)=3.23 ; ϵ (traj)= 107.61796 ; σ (traj)= 3.27750 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00

Pot a68 : (From Pot a00_1) Increase of 27% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 20.6% of ε (traj), Reduction of 22.9% of σ (traj)

 ϵ (ON)= 55.76 ; σ (ON)=3.23 ; ϵ (traj)= 111.41624 ; σ (traj)= 3.27750 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00

Pot a69 : (From Pot a00_1) Increase of 33.7% of ϵ (ON), Reduction of 20.6% of ϵ (traj), Reduction of 22.9% of σ (traj) ϵ (ON)= 58.69 ; σ (ON)=3.15 ; ϵ (traj)= 111.41624 ; σ (traj)= 3.27750 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00

Pot a70 : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 7.3% of σ (ON), Reduction of 20.6% of ε (traj), Reduction of 25.6% of σ (traj)

 ϵ (ON)= 58.69 ; σ (ON)=3.23 ; ϵ (traj)= 111.41624 ; σ (traj)= 3.20657 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00

Pot a71 : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 5.1% of σ (ON), Reduction of 20.6% of ε (traj), Reduction of 28.4% of σ (traj)

 ϵ (ON)= 58.69 ; σ (ON)=3.31 ; ϵ (traj)= 111.41624 ; σ (traj)= 3.13717 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00

Pot a72 : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 7.9% of σ (ON), Reduction of 20.6% of ε (traj), Reduction of 31.2% of σ (traj)

 ϵ (ON)= 58.69 ; σ (ON)=3.40 ; ϵ (traj)= 111.41624 ; σ (traj)= 3.06928 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00

Pot a39 –Figure 6 of publication : (From Pot a00_1) Increase of 33.7% of ε (ON), Increase of 2.5% of σ (ON), Reduction of 24.6% of ε (traj), Reduction of 18.6% of σ (traj)

 ϵ (ON)= 58.69 ; σ (ON)=3.23 ; ϵ (traj)= 101.29 ; σ (traj)= 3.2775 quadrupole moment in 10^-26 esu = 1.8490 1.8490 -3.6980 vibrational dependence of polarizability 0.263900E+010.140000E+000.700000E-010.268000E+00

