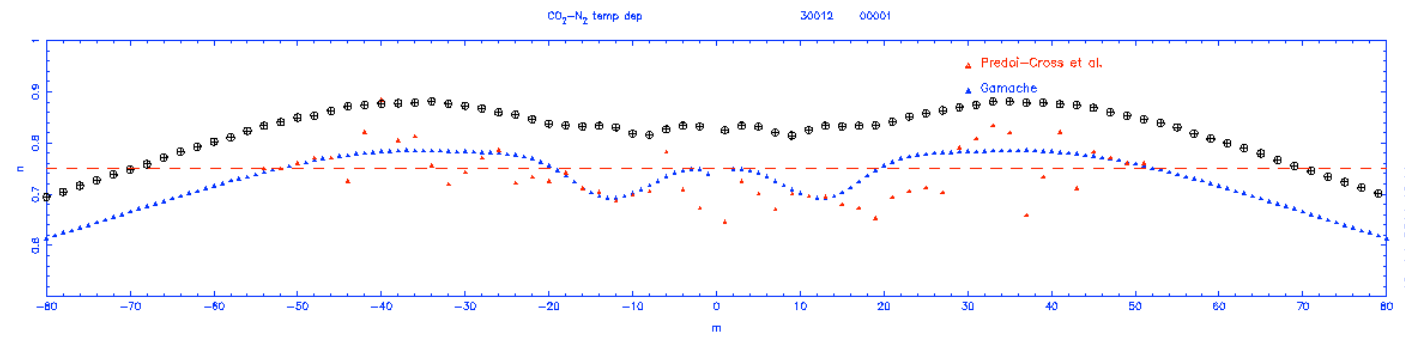
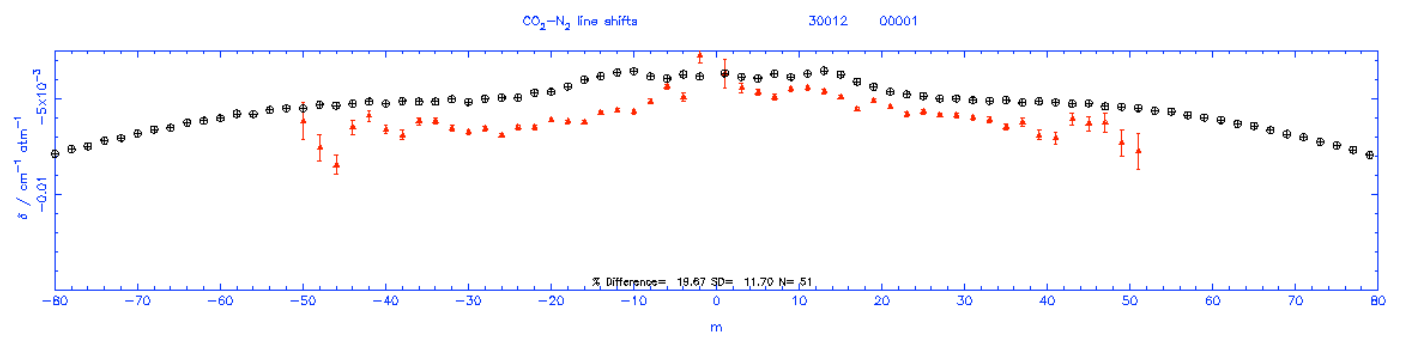
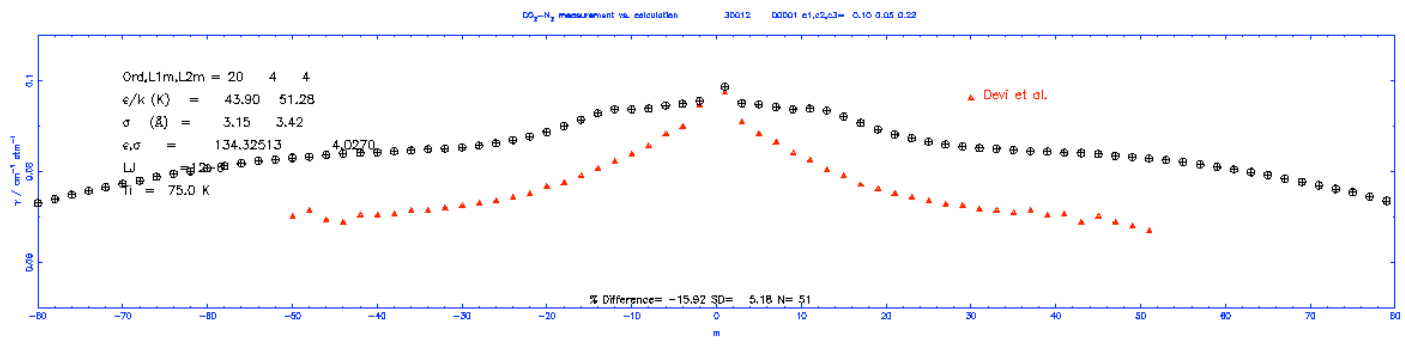


Pot a00_1 : Initial calculations – See plot for the values of the atom-atom parameters

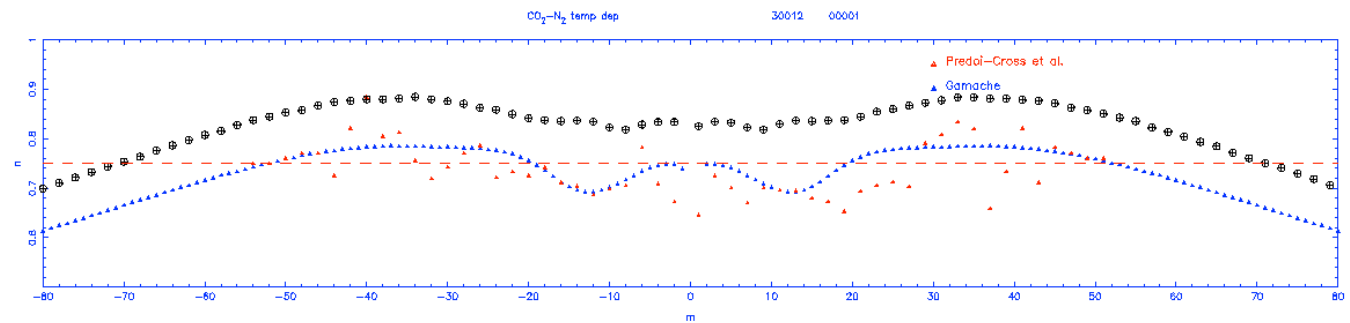
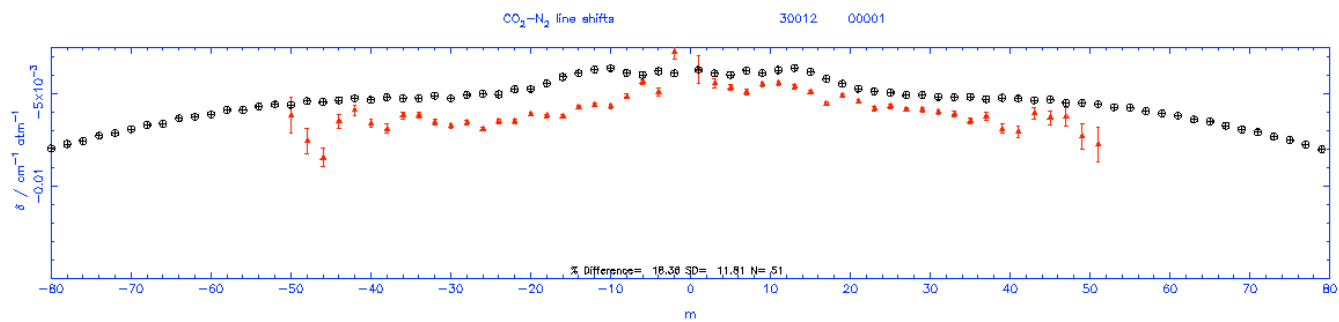
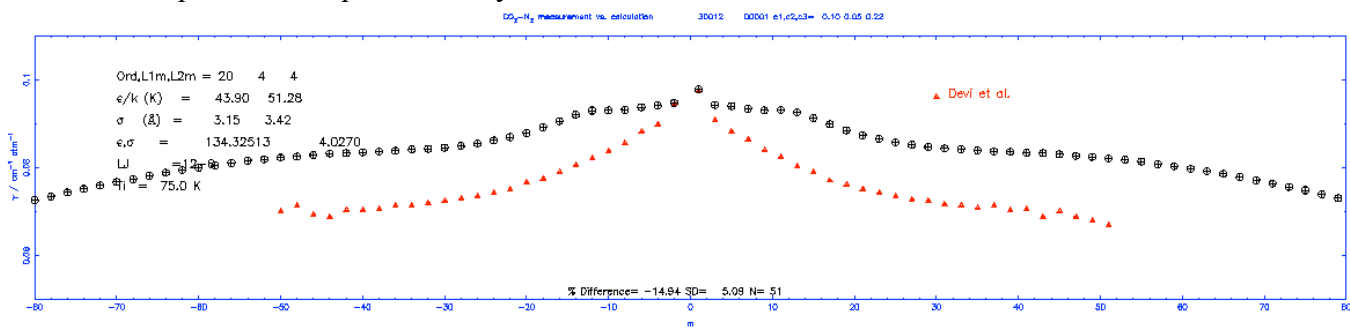
quadrupole moment in 10^{-26} esu = 2.0100 2.0100 -4.0200

vibrational dependence of polarizability : 0.263900E+010.100000E+000.516000E-010.223600E+00



19-Jul-2011 19:14

Pot a00_2 : Pot a00_1 with a reduction of 5% of the quadrupole moment of CO₂
 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

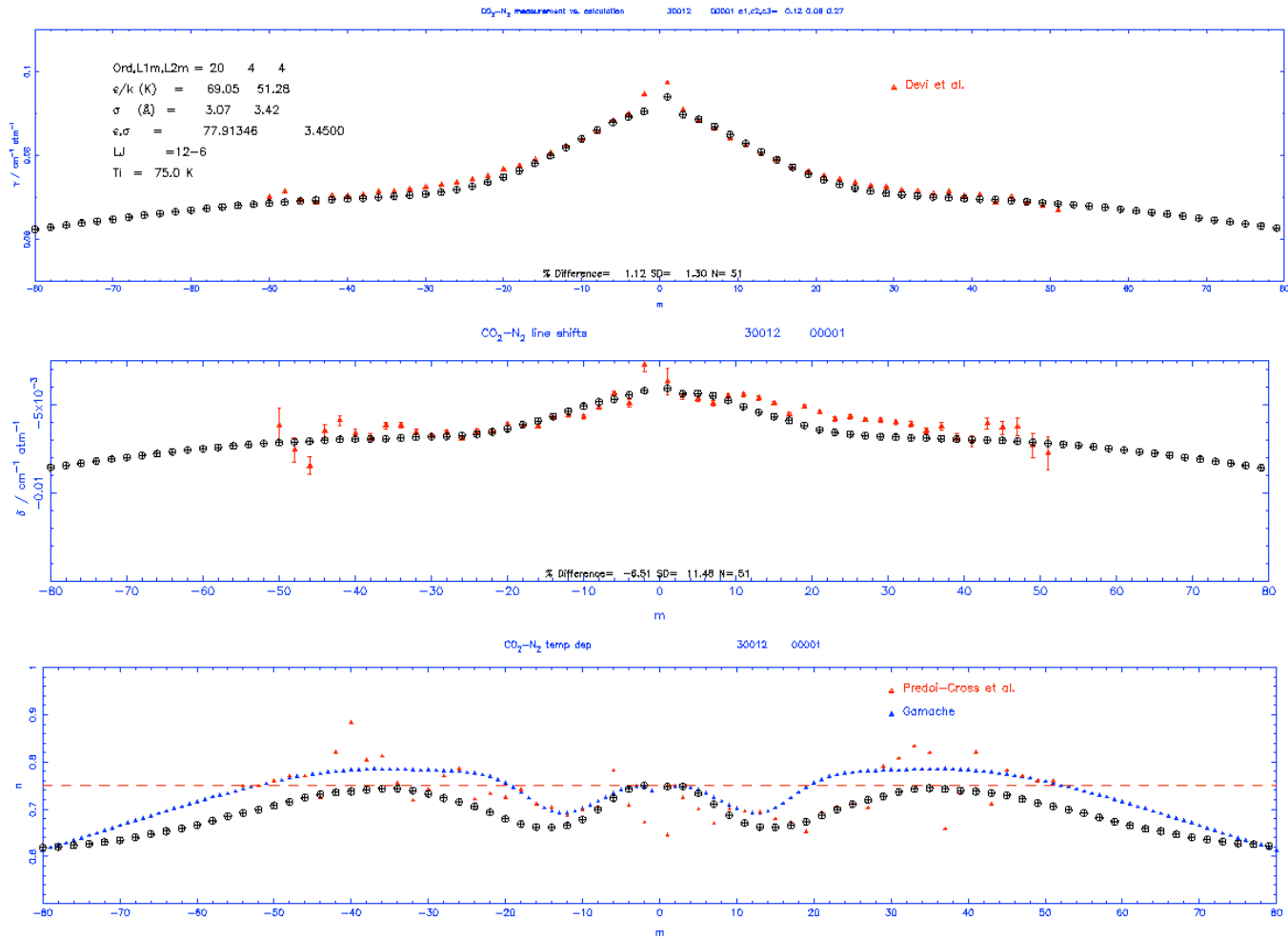


19-Jul-2011 19:15

Pot a25_1 : (From Pot a00_1) Increase of 60% of $\epsilon(\text{ON})$, Reduction of 2.6% of $\sigma(\text{ON})$, Reduction of 72% of $\epsilon(\text{traj})$, Reduction of 17% of $\sigma(\text{traj})$

quadrupole moment in 10^{-26} esu = 1.8900 1.8900 -3.7800

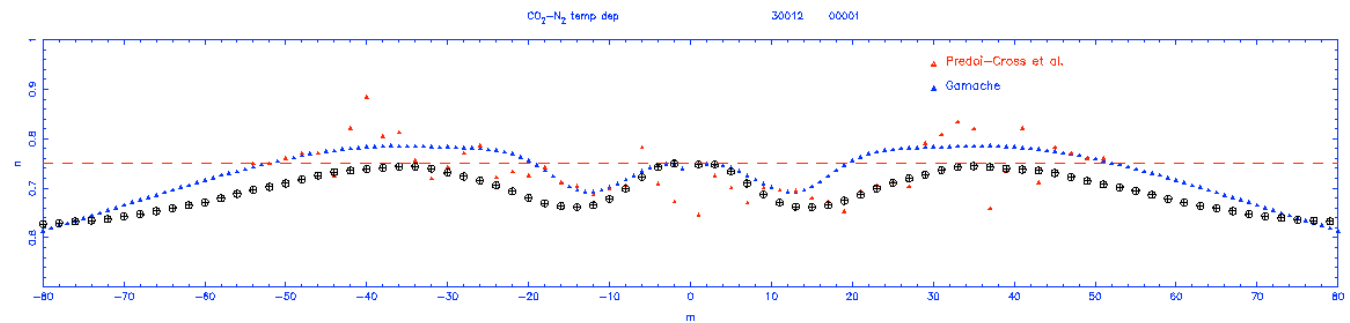
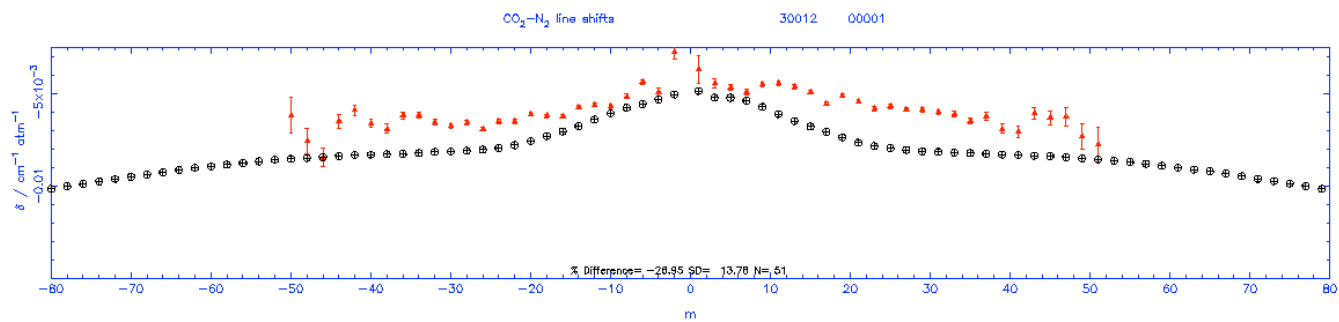
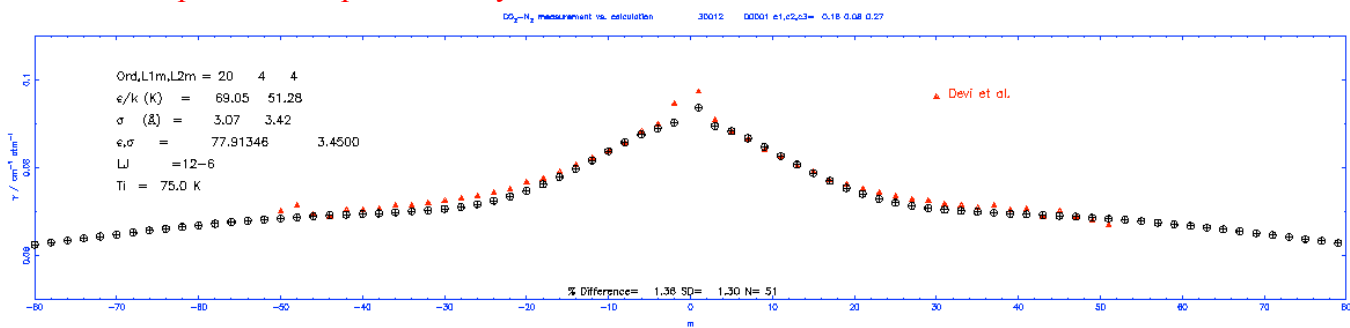
vibrational dependence of polarizability 0.263900E+01 0.120000E+00 0.618000E-01 0.268000E+00



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

quadrupole moment in 10⁻²⁶ esu = 1.8490 1.8490 -3.6980

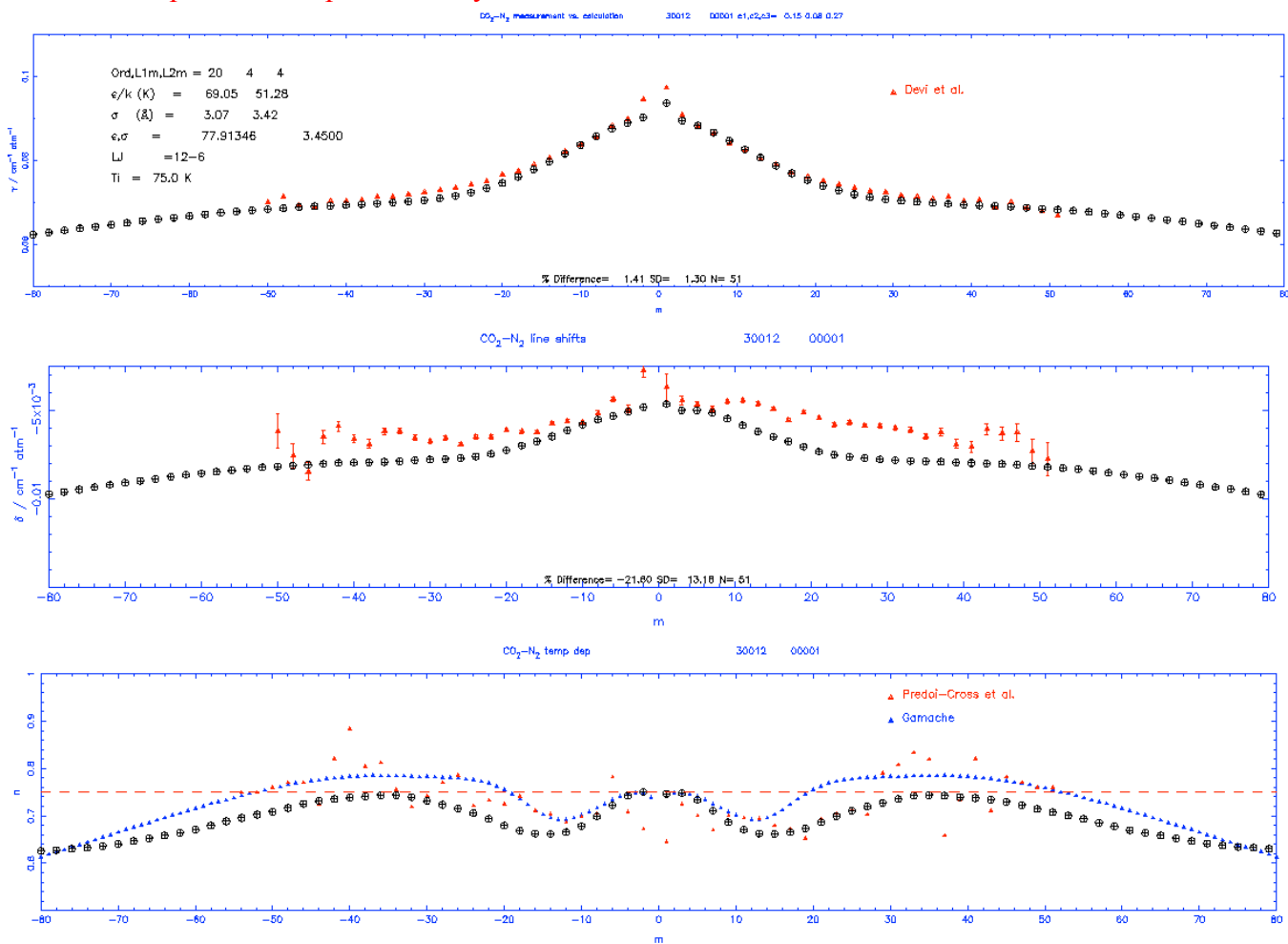
vibrational dependence of polarizability 0.263900E+01 0.160000E+00 0.810000E-01 0.268000E+00



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

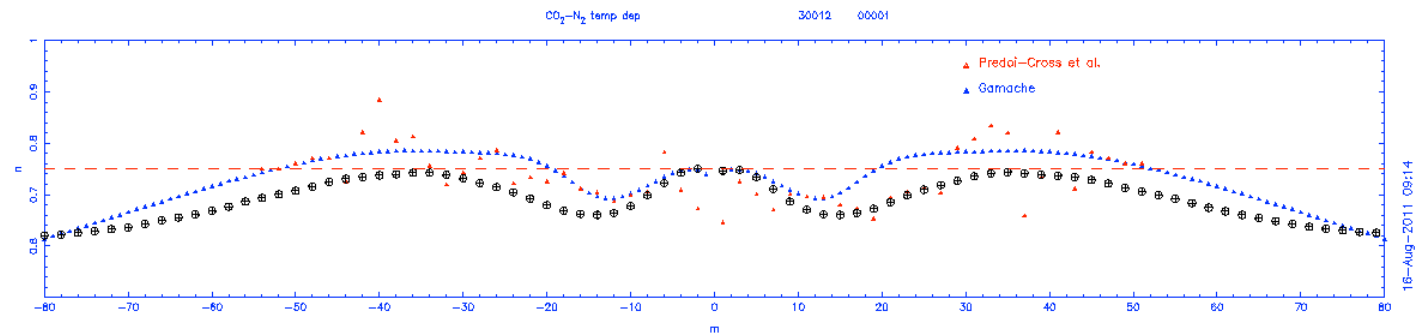
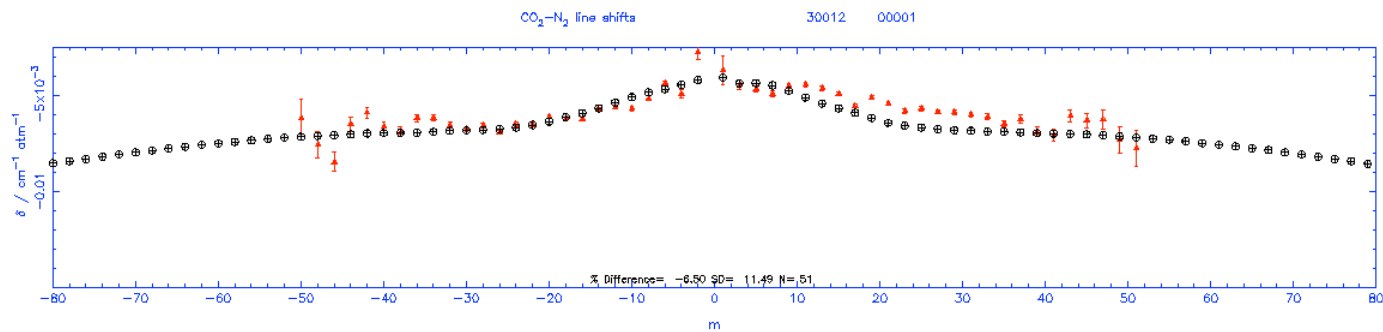
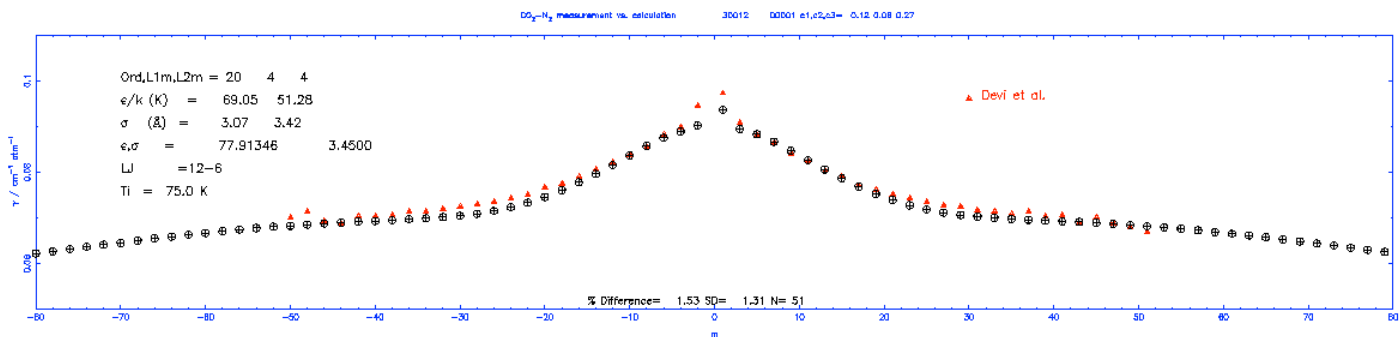
vibrational dependence of polarizability 0.263900E+01 0.150000E+00 0.750000E-01 0.268000E+00



Pot a25_4 : Pot a25_1 with a reduction of 2.2% of the quadrupole moment of CO₂

quadrupole moment in 10⁻²⁶ esu = 1.8490 1.8490 -3.6980

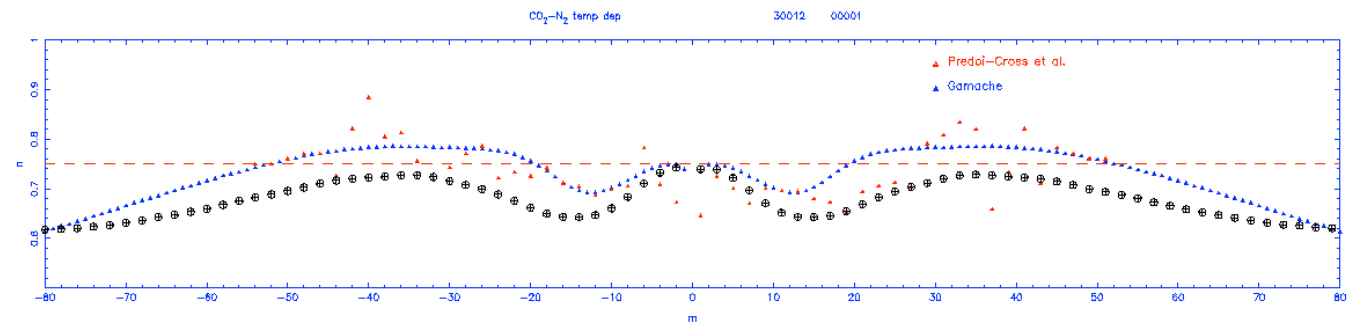
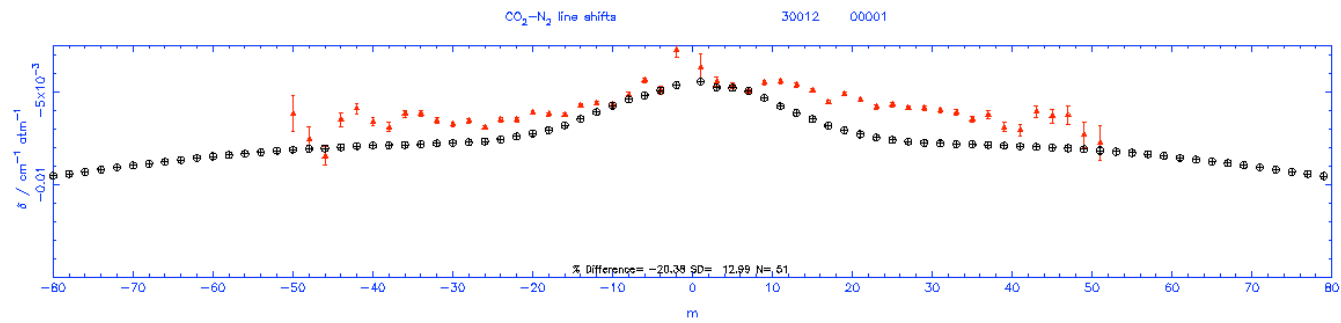
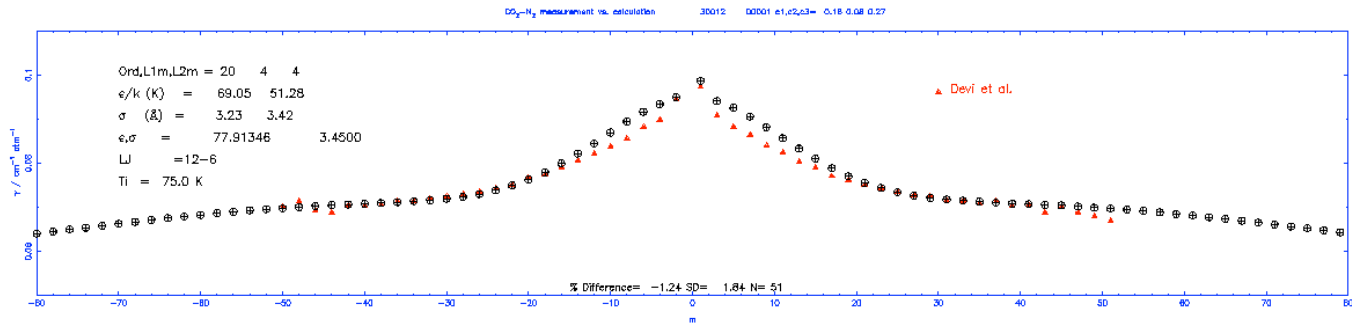
vibrational dependence of polarizability 0.263900E+010.120000E+000.600000E-010.268000E+00



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

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

vibrational dependence of polarizability 0.263900E+01 0.160000E+00 0.810000E-01 0.268000E+00

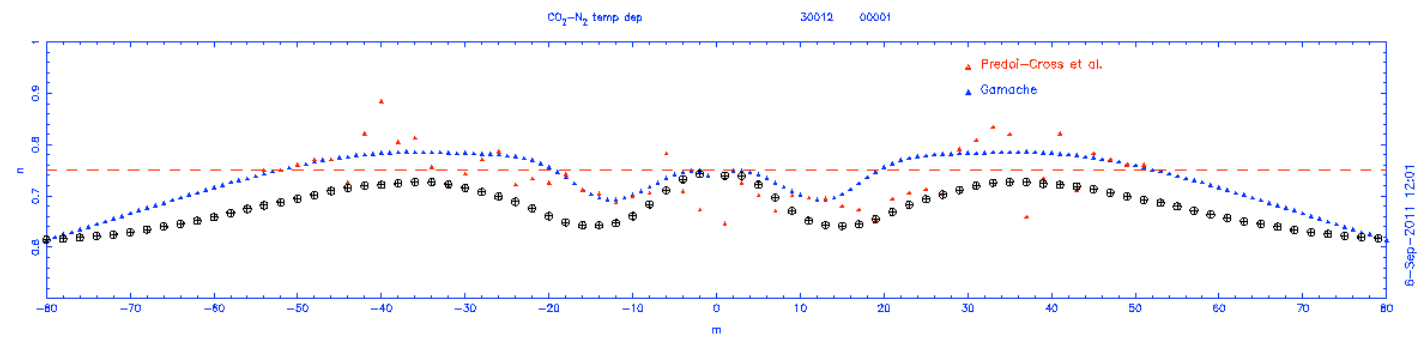
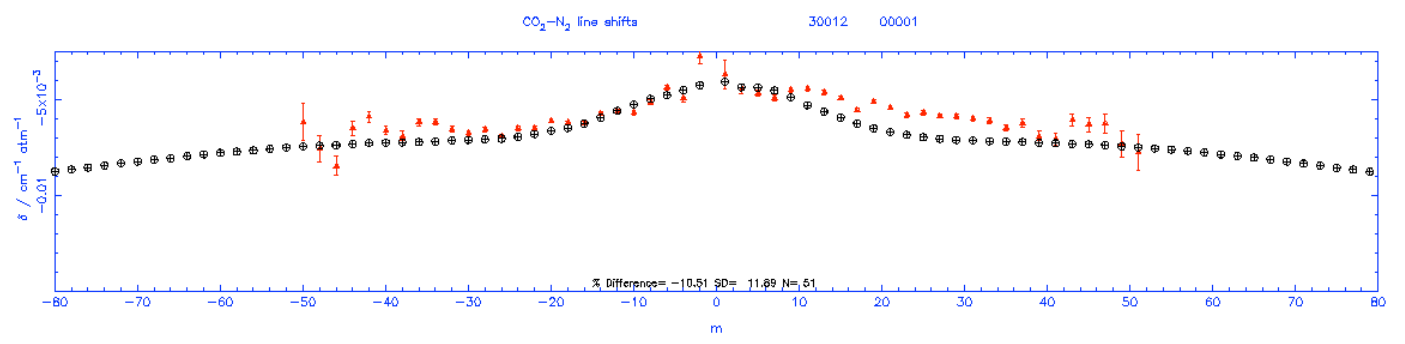
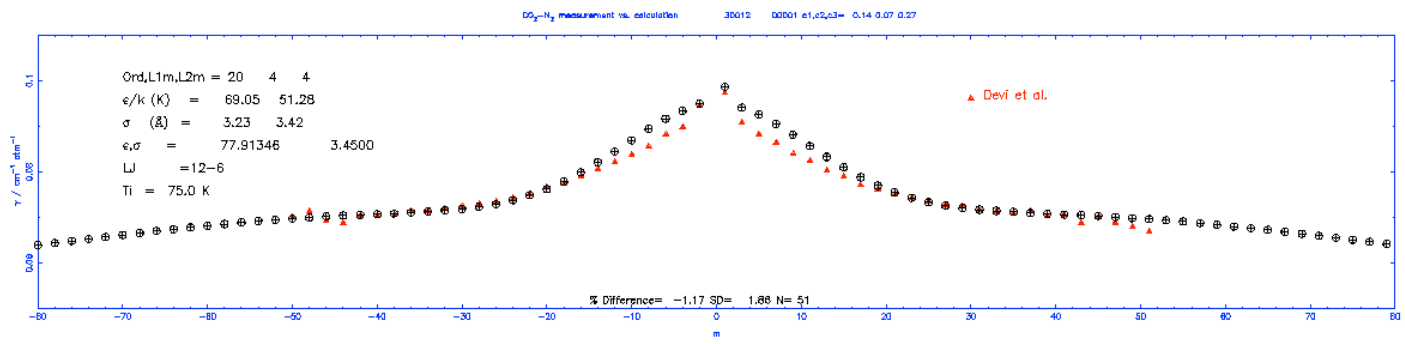


3-Aug-2011 11:17

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 -3.6980

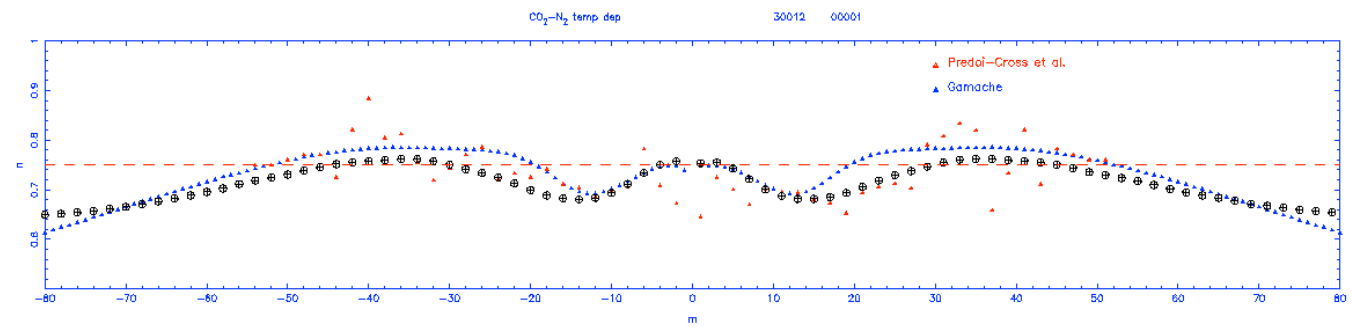
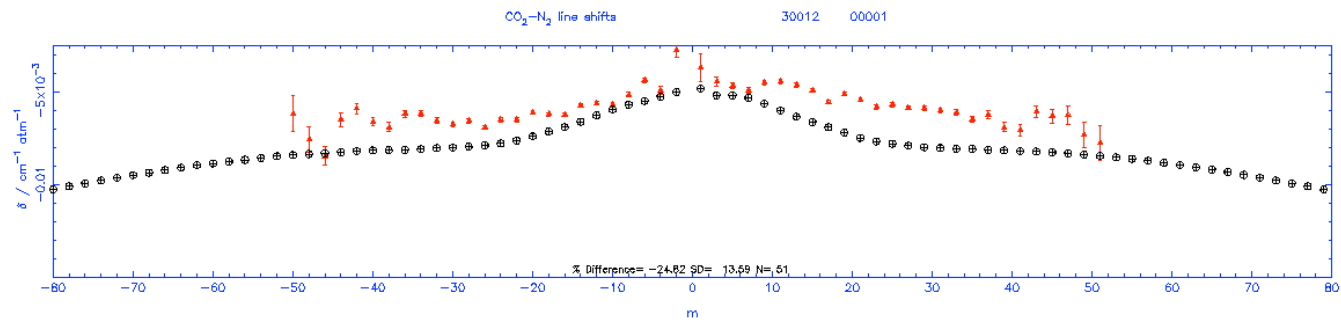
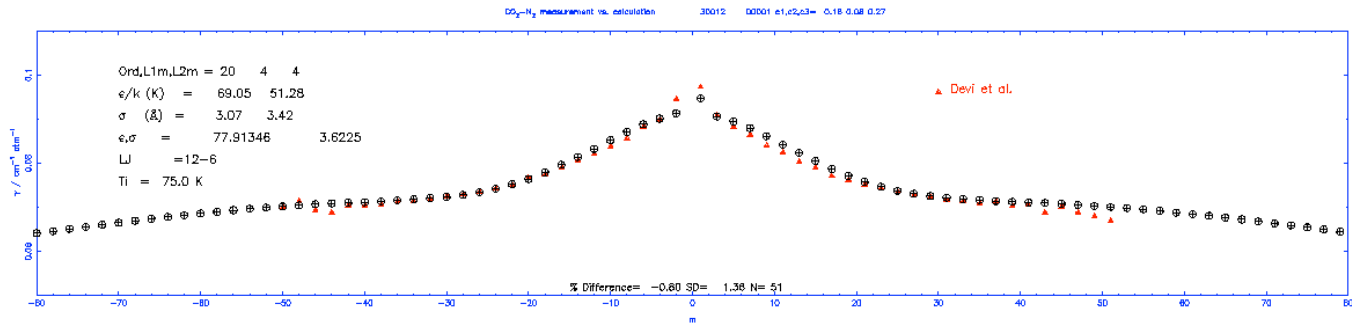
vibrational dependence of polarizability $0.263900E+01$ $0.140000E+00$ $0.700000E-01$ $0.268000E+00$



Pot a27_1 : (From Pot a00_1) Increase of 60% of $\epsilon(\text{ON})$, Reduction of 2.6% of $\sigma(\text{ON})$, Reduction of 72% of $\epsilon(\text{traj})$, Reduction of 11% of $\sigma(\text{traj})$

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

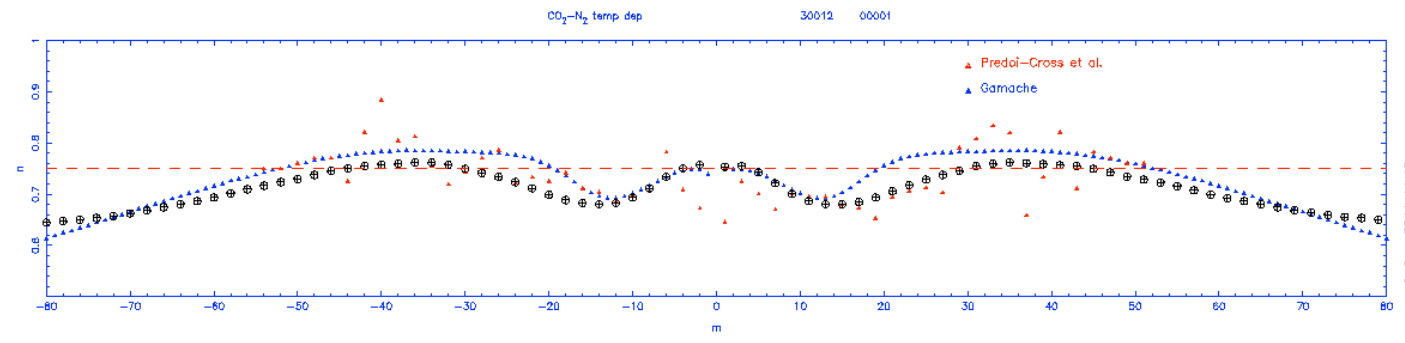
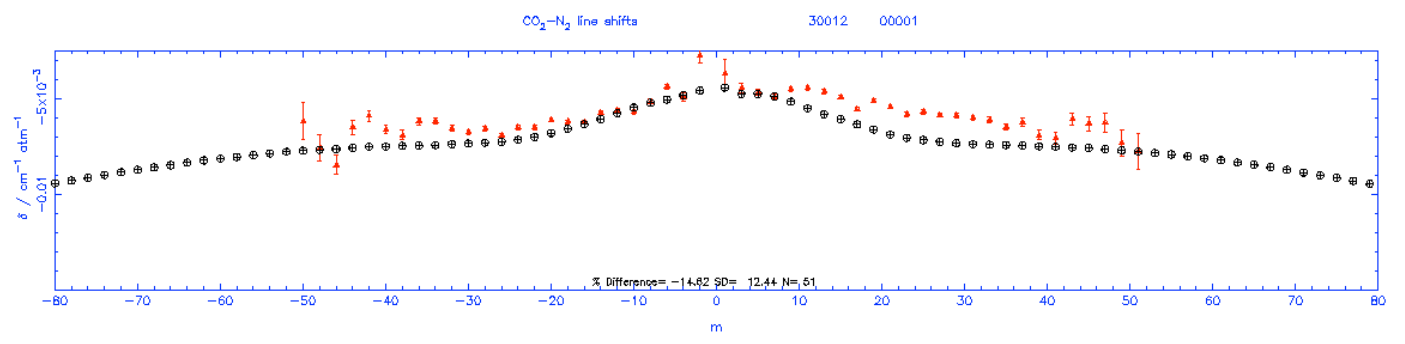
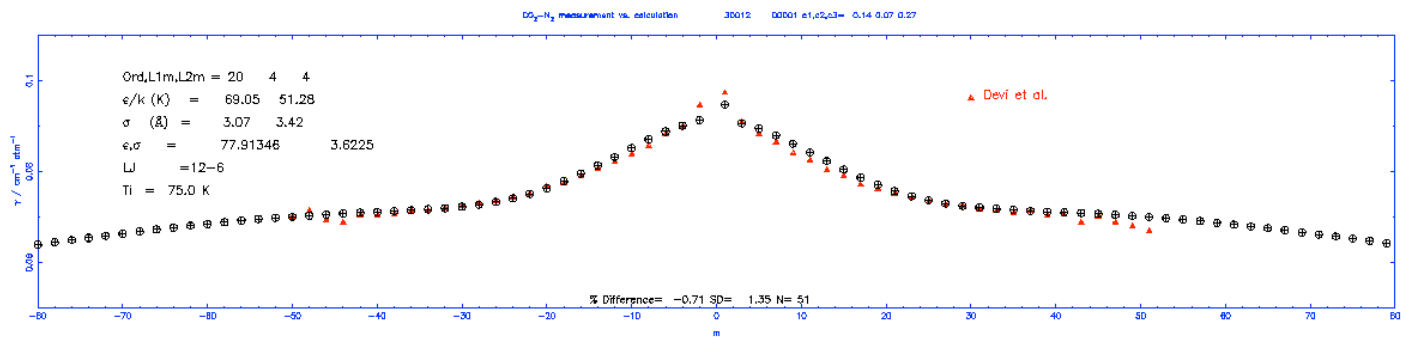
vibrational dependence of polarizability $0.263900\text{E}+010.160000\text{E}+000.810000\text{E}-010.268000\text{E}+00$



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

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

vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00

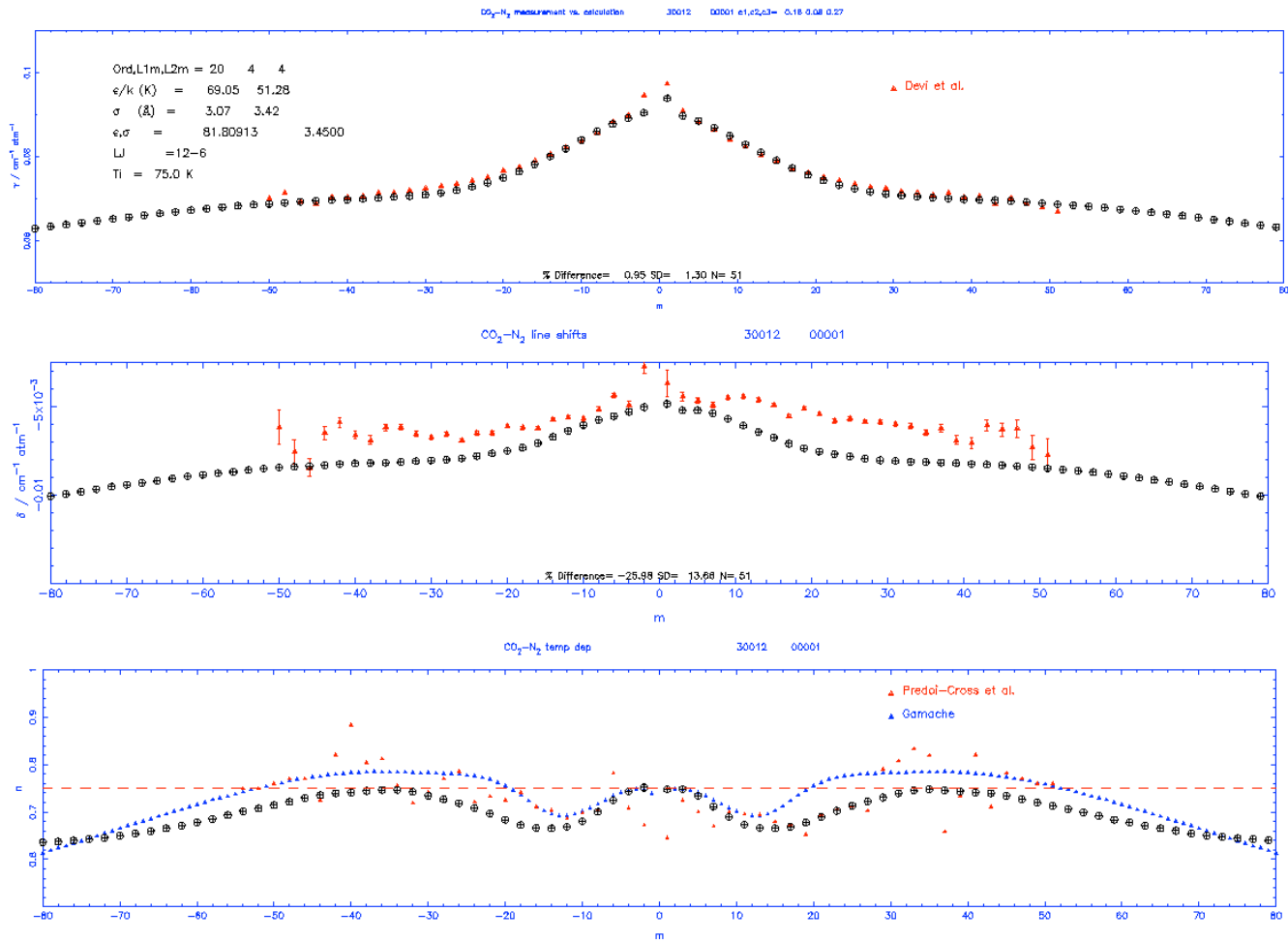


6-Sep-2011 11:45

Pot a28 : (From Pot a00_1) Increase of 60% of $\epsilon(\text{ON})$, Reduction of 2.6% of $\sigma(\text{ON})$, Reduction of 64% of $\epsilon(\text{traj})$, Reduction of 16.7% of $\sigma(\text{traj})$

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

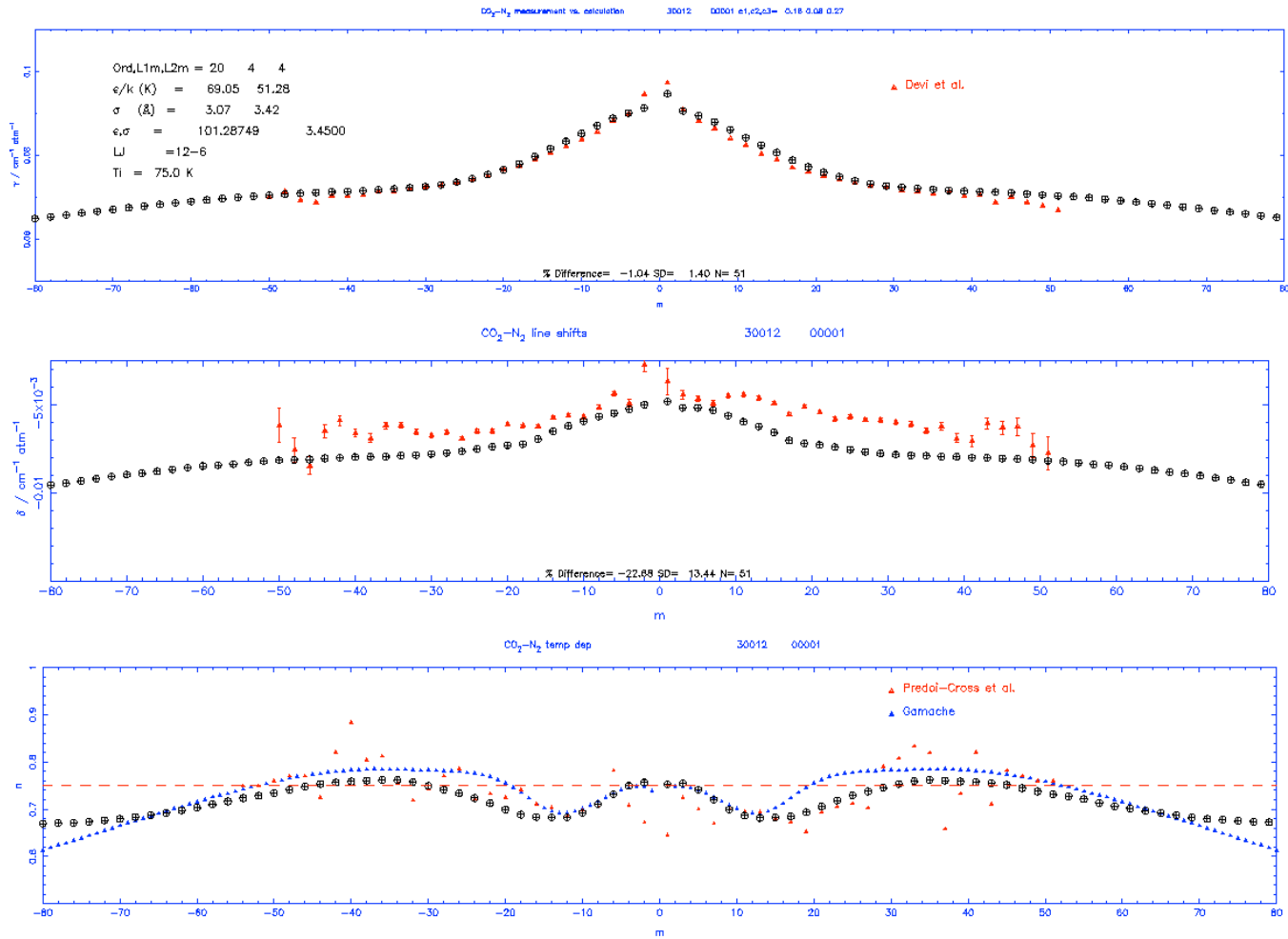
vibrational dependence of polarizability 0.263900E+01 0.160000E+00 0.810000E-01 0.268000E+00



Pot a29_1 : (From Pot a00_1) Increase of 60% of $\epsilon(\text{ON})$, Reduction of 2.6% of $\sigma(\text{ON})$, Reduction of 32.6% of $\epsilon(\text{traj})$, Reduction of 16.7% of $\sigma(\text{traj})$

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

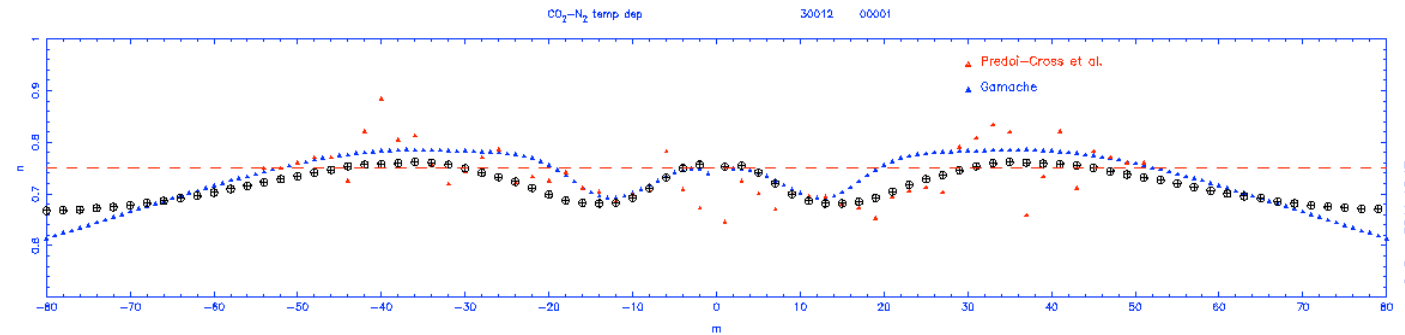
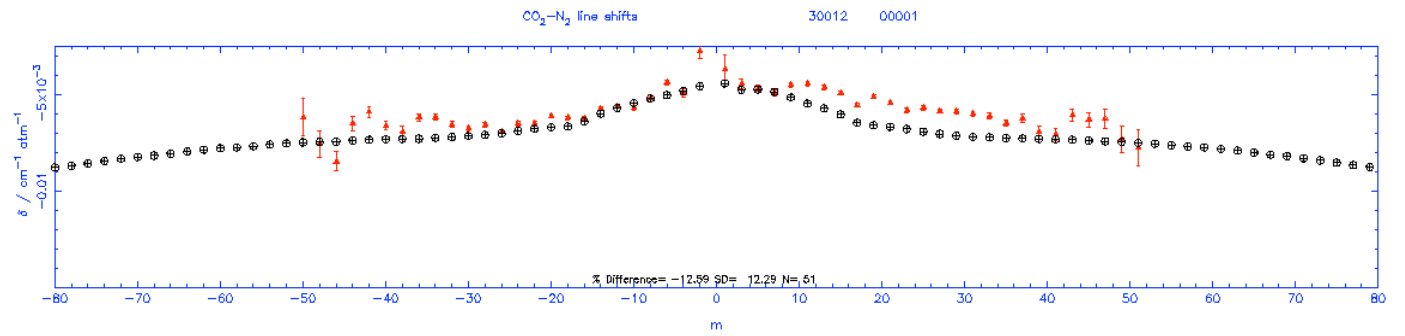
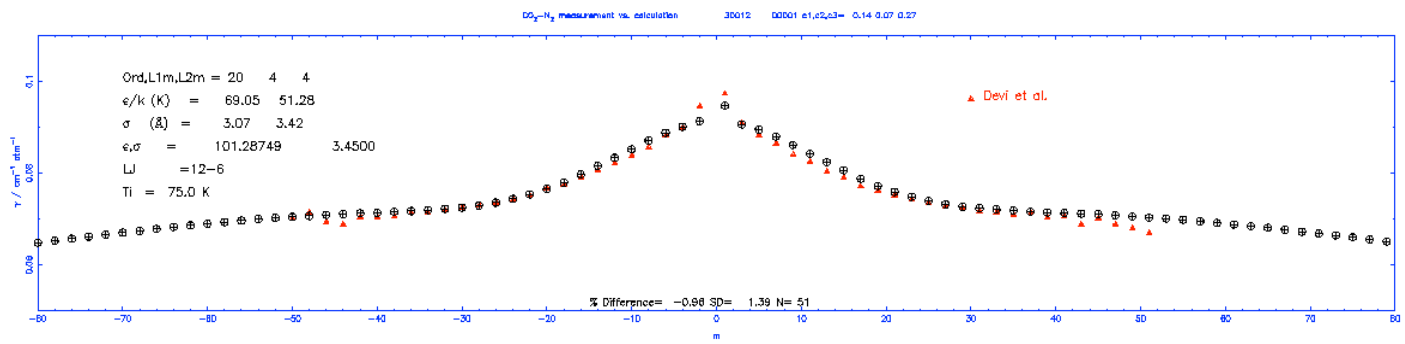
vibrational dependence of polarizability 0.263900E+01 0.160000E+00 0.810000E-01 0.268000E+00



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 -3.6980

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

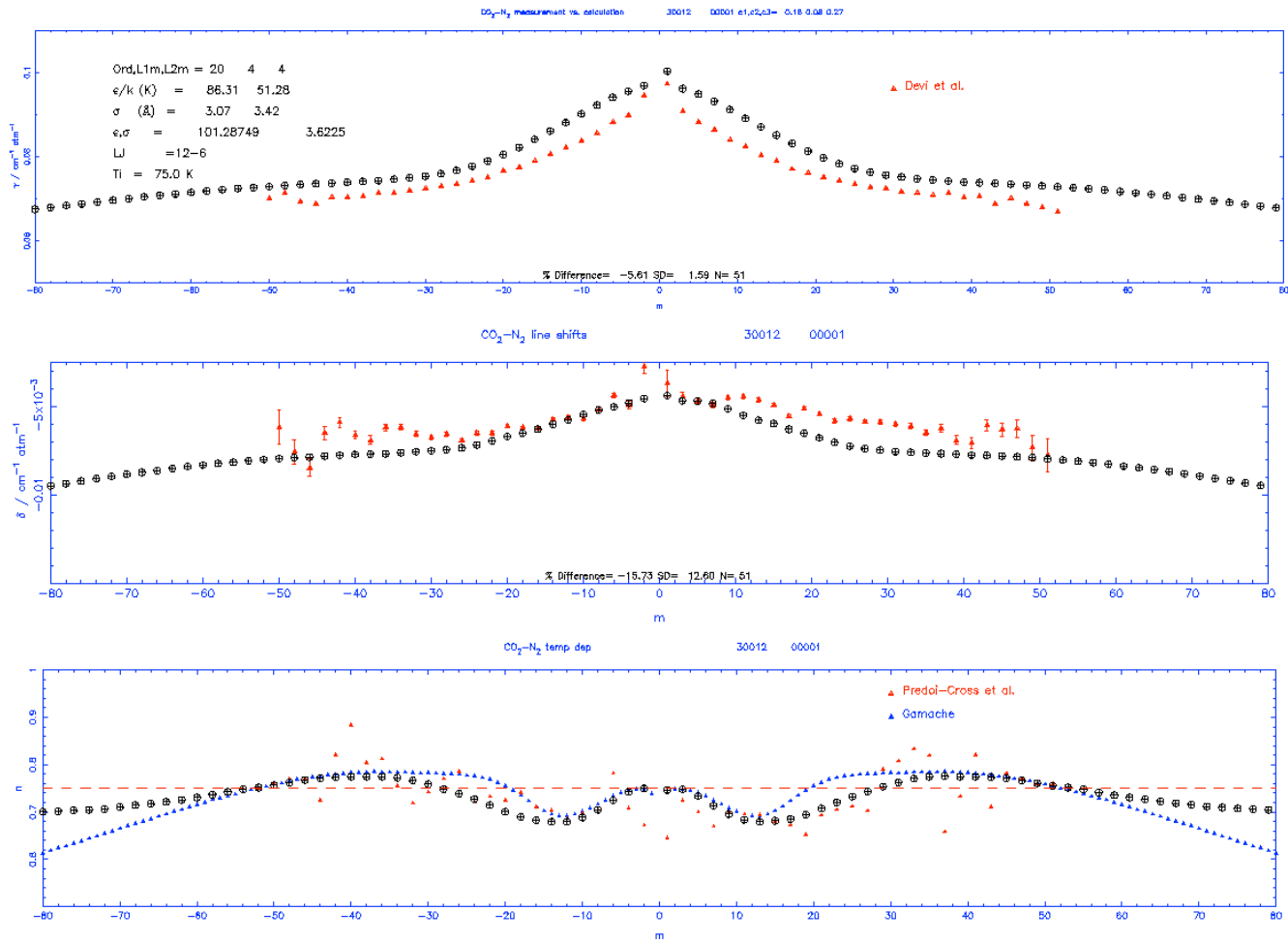


6-Sep-2011 12:17

Pot a30 : (From Pot a00_1) Increase of 96.6% of $\epsilon(\text{ON})$, Reduction of 2.6% of $\sigma(\text{ON})$, Reduction of 32.6% of $\epsilon(\text{traj})$, Reduction of 11% of $\sigma(\text{traj})$

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

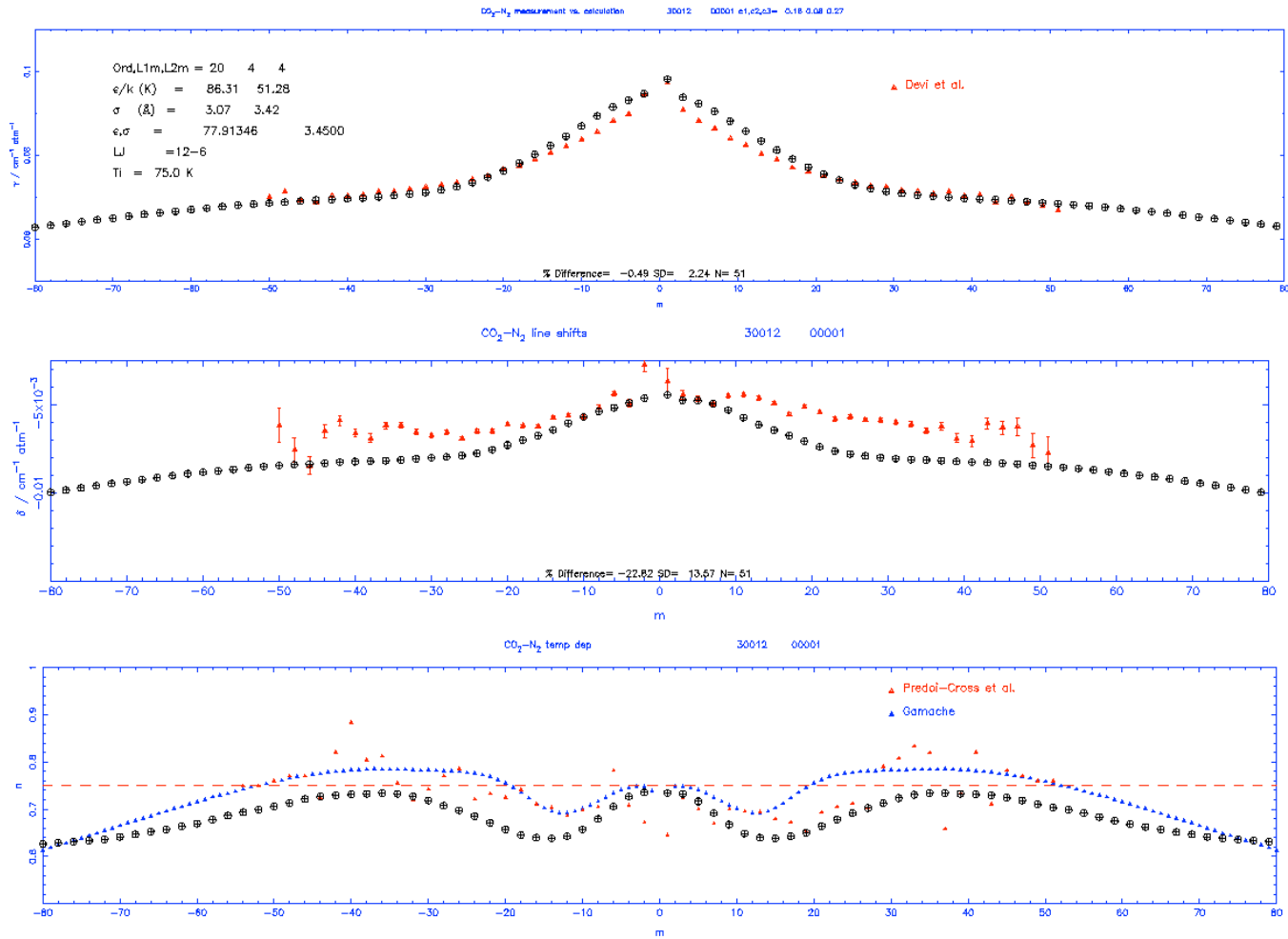
vibrational dependence of polarizability 0.263900E+01 0.160000E+00 0.810000E-01 0.268000E+00



Pot a31_1 : (From Pot a00_1) Increase of 96.6% of $\epsilon(\text{ON})$, Reduction of 2.6% of $\sigma(\text{ON})$, Reduction of 72% of $\epsilon(\text{traj})$, Reduction of 11% of $\sigma(\text{traj})$

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

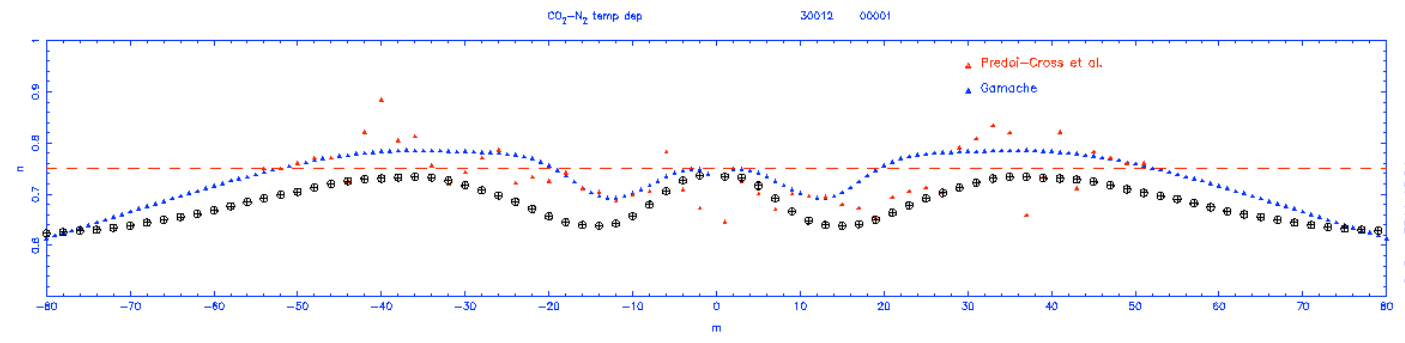
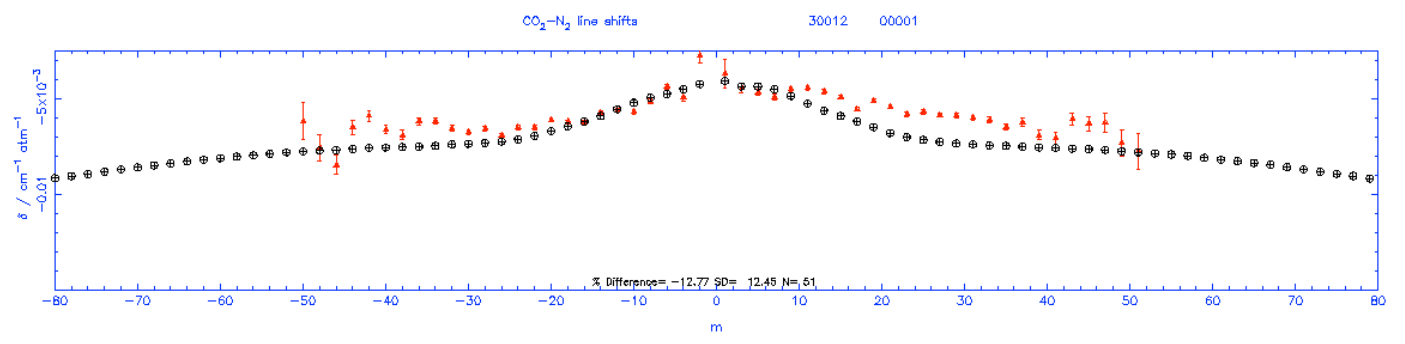
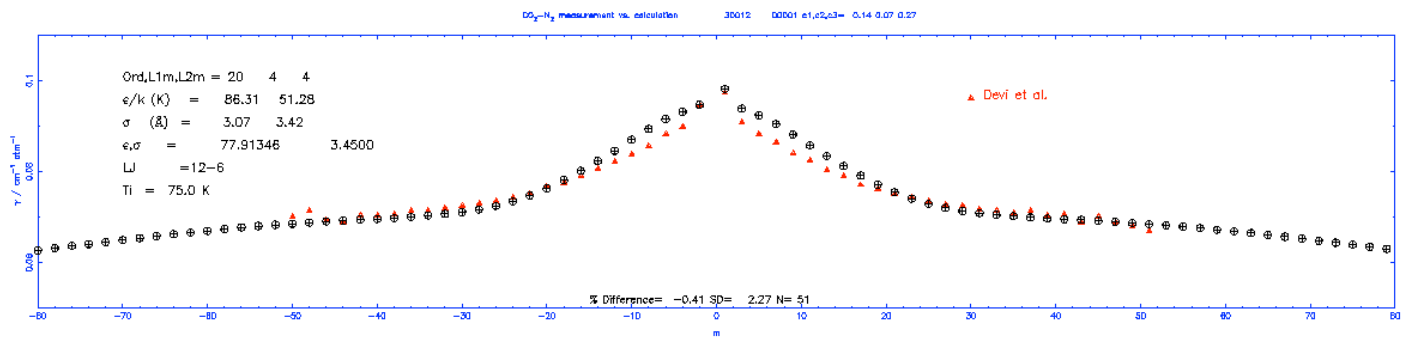
vibrational dependence of polarizability 0.263900E+01 0.160000E+00 0.810000E-01 0.268000E+00



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

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

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

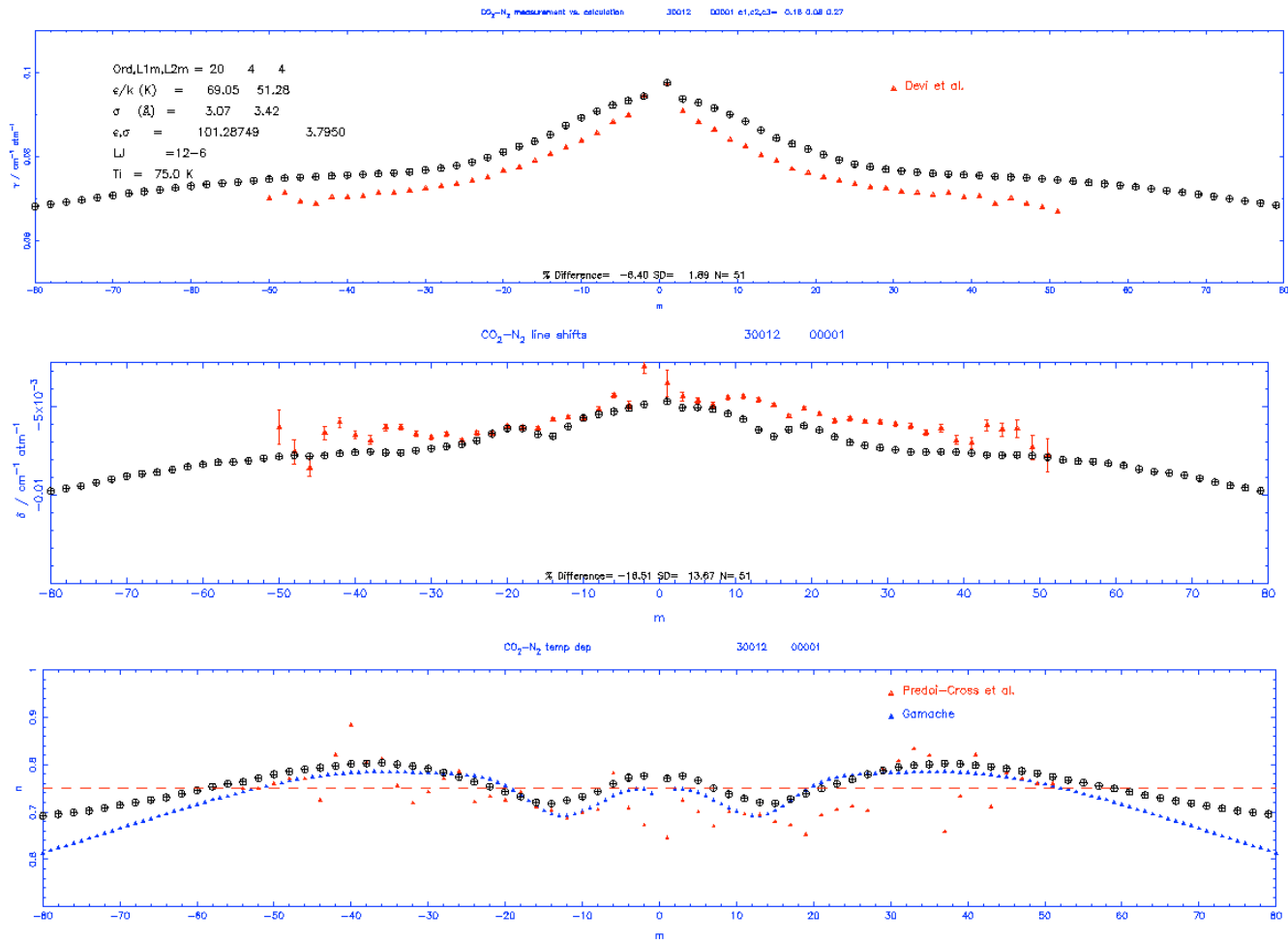


6-Sep-2011 15:04

Pot a32 : (From Pot a00_1) Increase of 57.3% of $\epsilon(\text{ON})$, Reduction of 2.6% of $\sigma(\text{ON})$, Reduction of 32.6% of $\epsilon(\text{traj})$, Reduction of 6.1% of $\sigma(\text{traj})$

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

vibrational dependence of polarizability 0.263900E+01 0.160000E+00 0.810000E-01 0.268000E+00

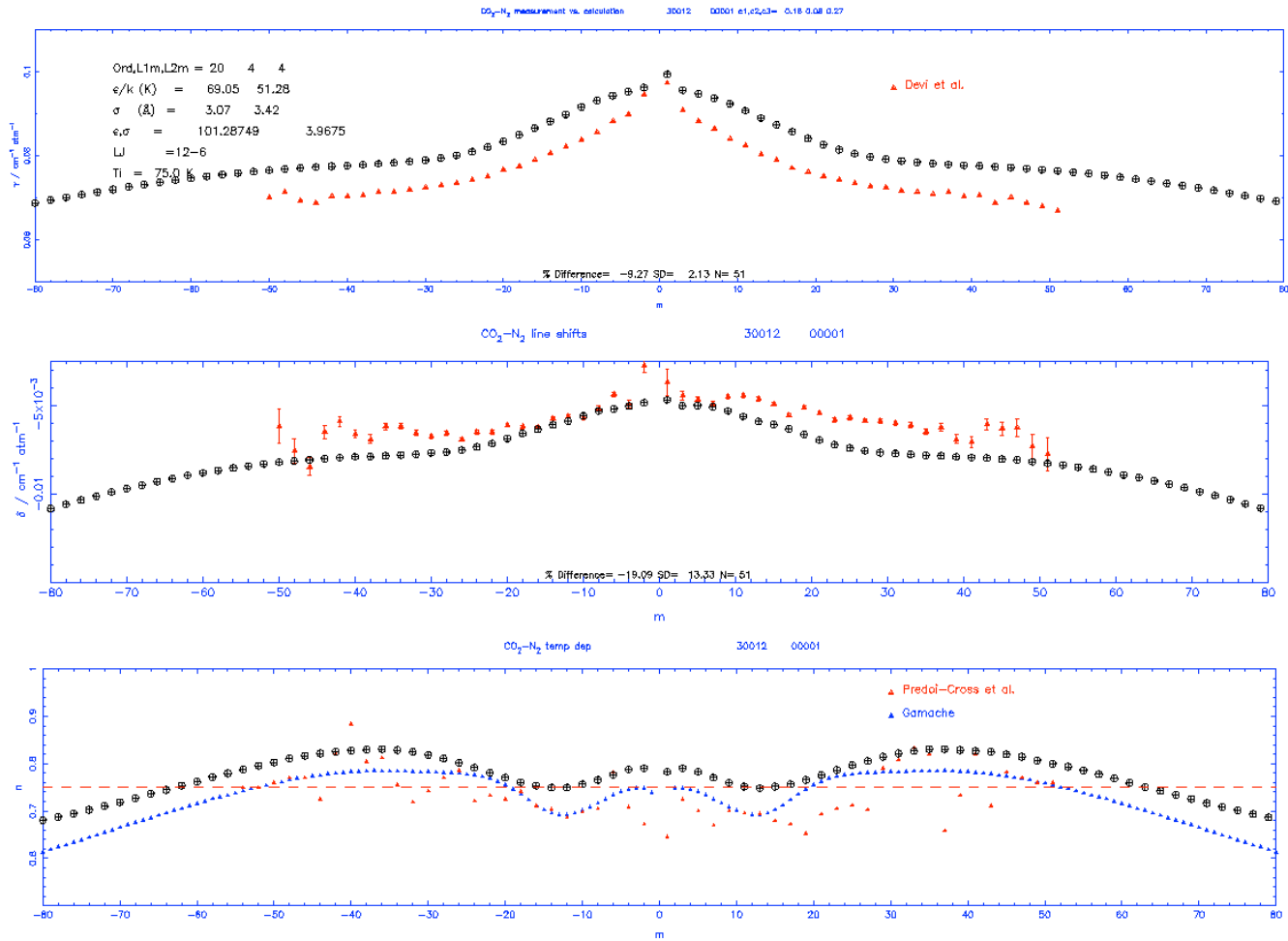


4-Aug-2011 17:46

Pot a33 : (From Pot a00_1) Increase of 57.3% of $\epsilon(\text{ON})$, Reduction of 2.6% of $\sigma(\text{ON})$, Reduction of 32.6% of $\epsilon(\text{traj})$, Reduction of 1.5% of $\sigma(\text{traj})$

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

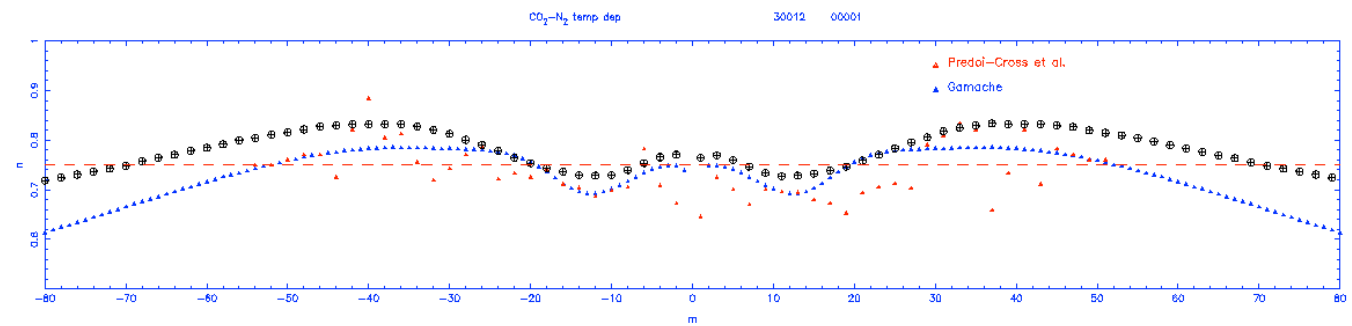
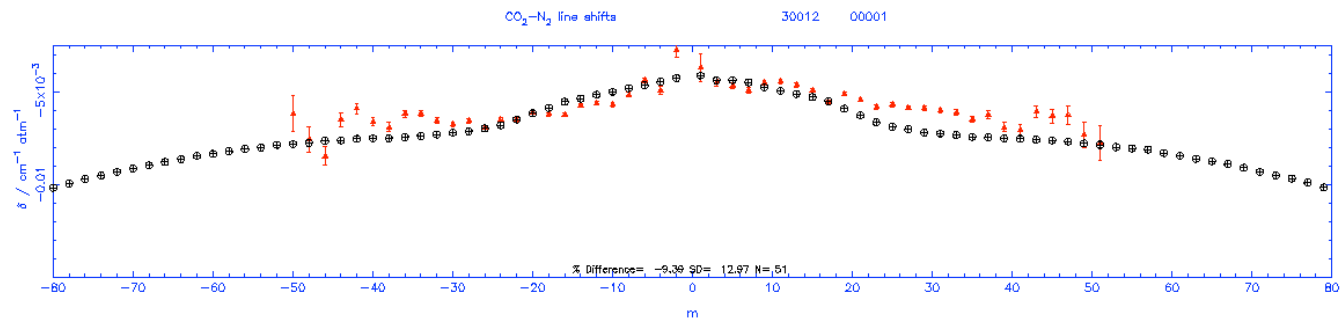
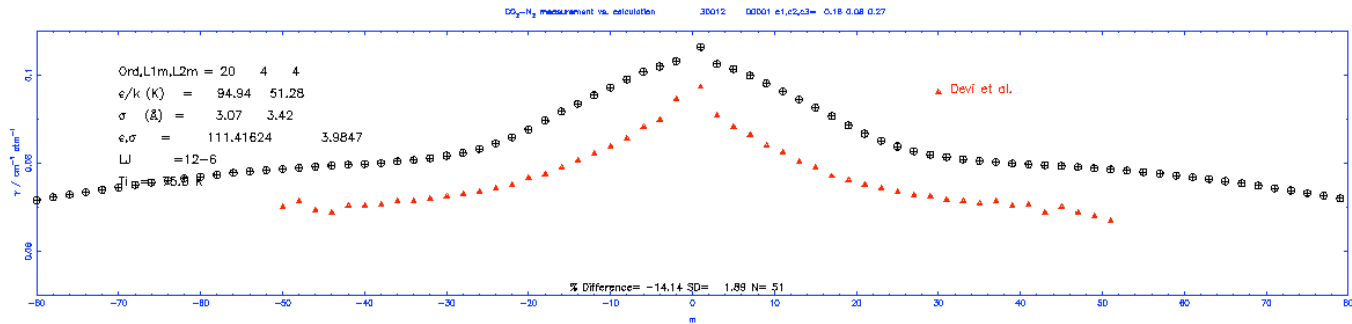
vibrational dependence of polarizability 0.263900E+01 0.160000E+00 0.810000E-01 0.268000E+00



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

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

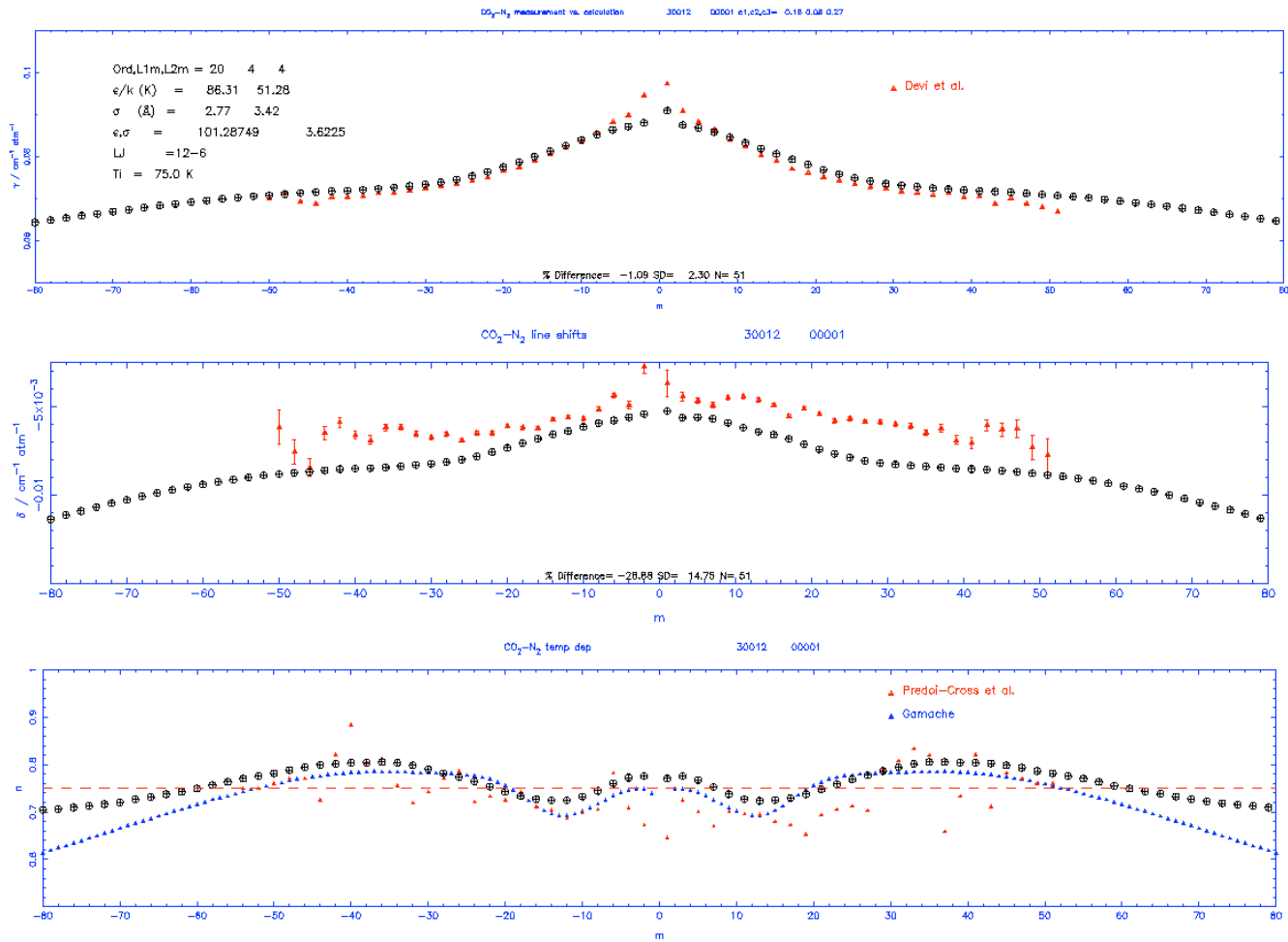
vibrational dependence of polarizability 0.263900E+01 0.160000E+00 0.810000E-01 0.268000E+00



Pot a35 : (From Pot a00_1) Increase of 49% of $\epsilon(\text{ON})$, Reduction of 2.6% of $\sigma(\text{ON})$, Reduction of 13.7% of $\epsilon(\text{traj})$, Reduction of 11% of $\sigma(\text{traj})$

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

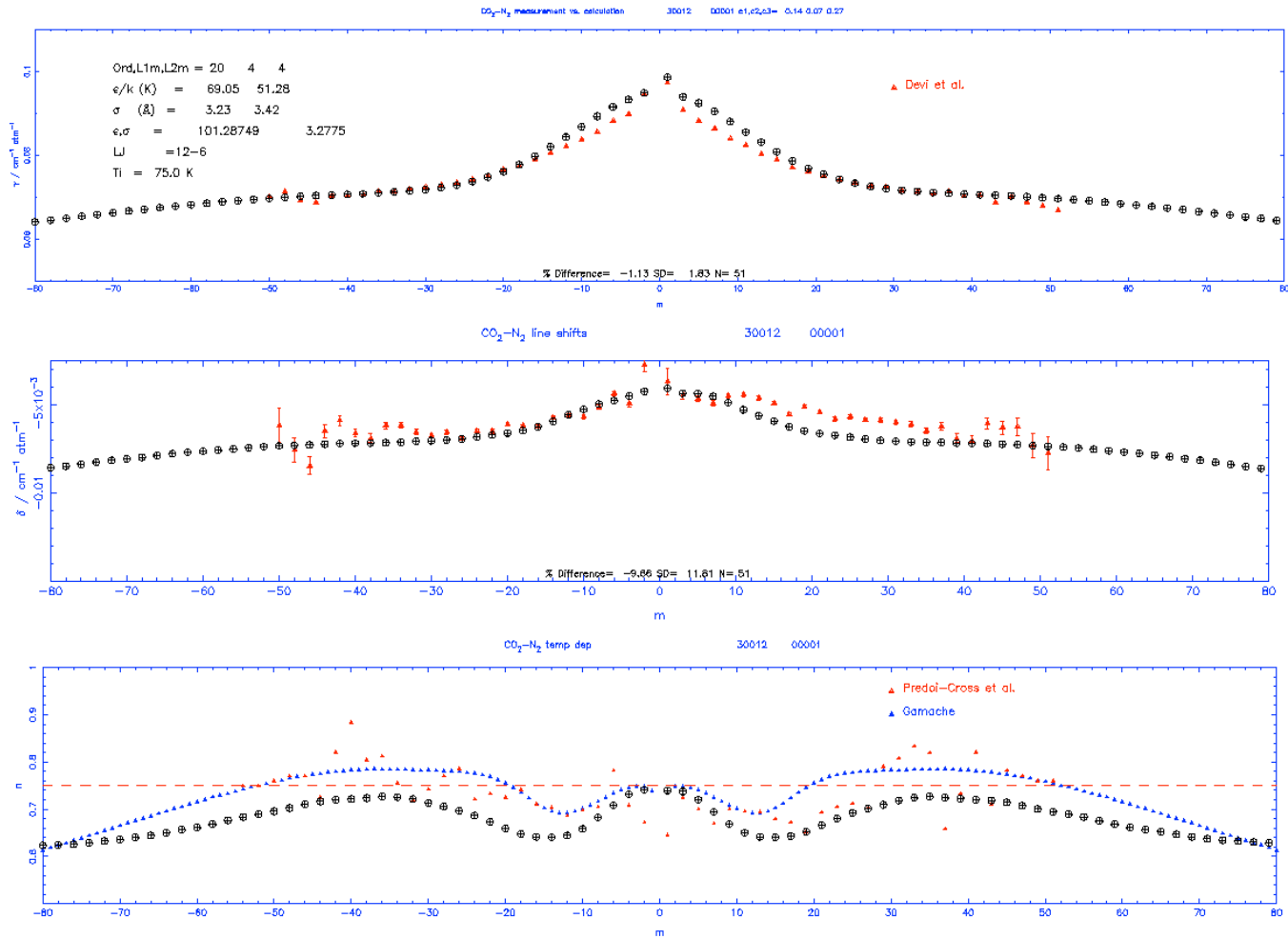
vibrational dependence of polarizability 0.263900E+01 0.160000E+00 0.810000E-01 0.268000E+00



Pot a38 : (From Pot a00_1) Increase of 57.3% of $\epsilon(\text{ON})$, Increase of 2.3% of $\sigma(\text{ON})$, Reduction of 32.6% of $\epsilon(\text{traj})$, Reduction of 22.9% of $\sigma(\text{traj})$

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

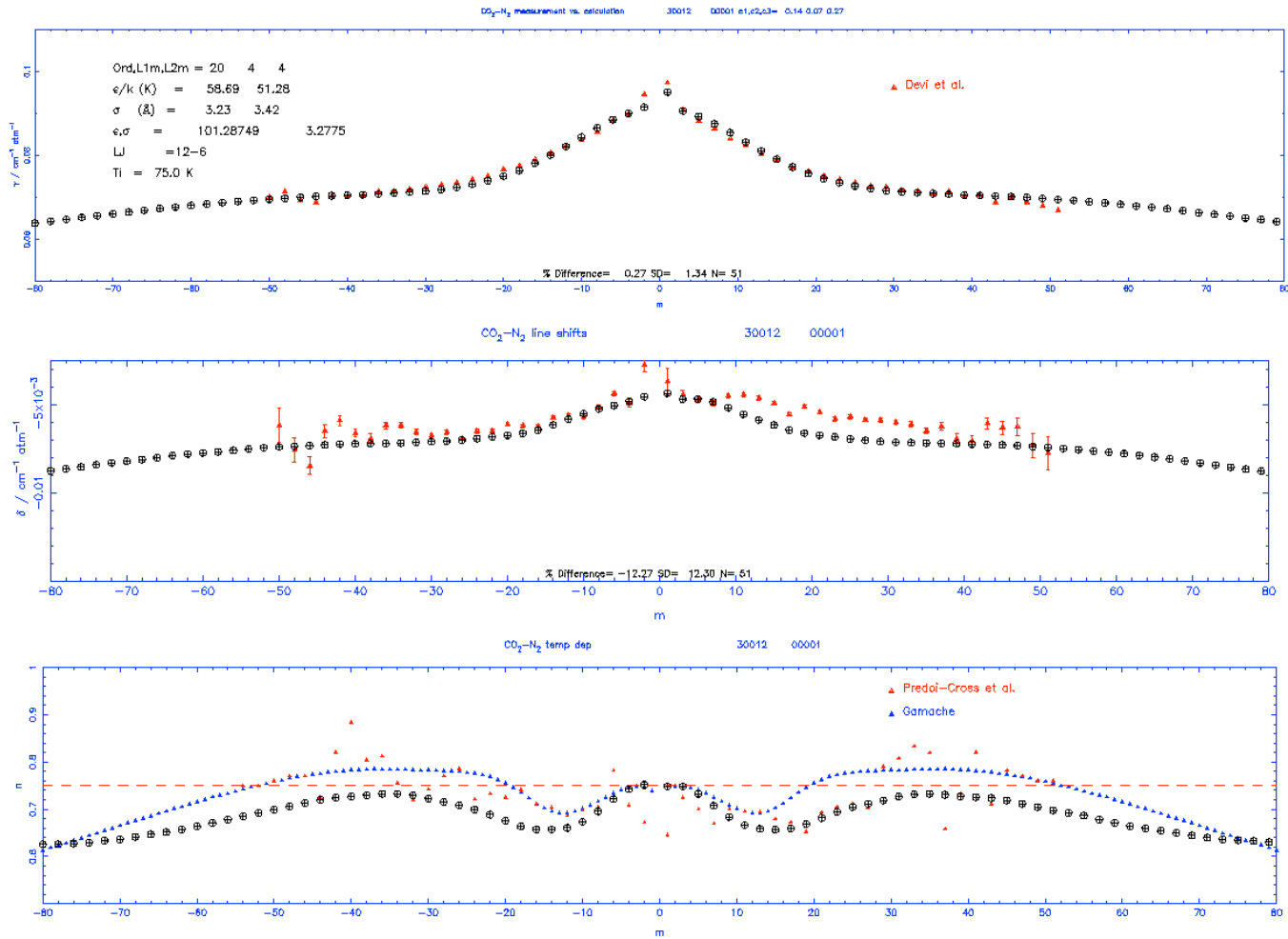
vibrational dependence of polarizability $0.263900\text{E}+010.140000\text{E}+000.700000\text{E}-010.268000\text{E}+00$



Pot a39 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 2.5% of $\sigma(\text{ON})$, Reduction of 32.6% of $\epsilon(\text{traj})$, Reduction of 22.9% of $\sigma(\text{traj})$

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

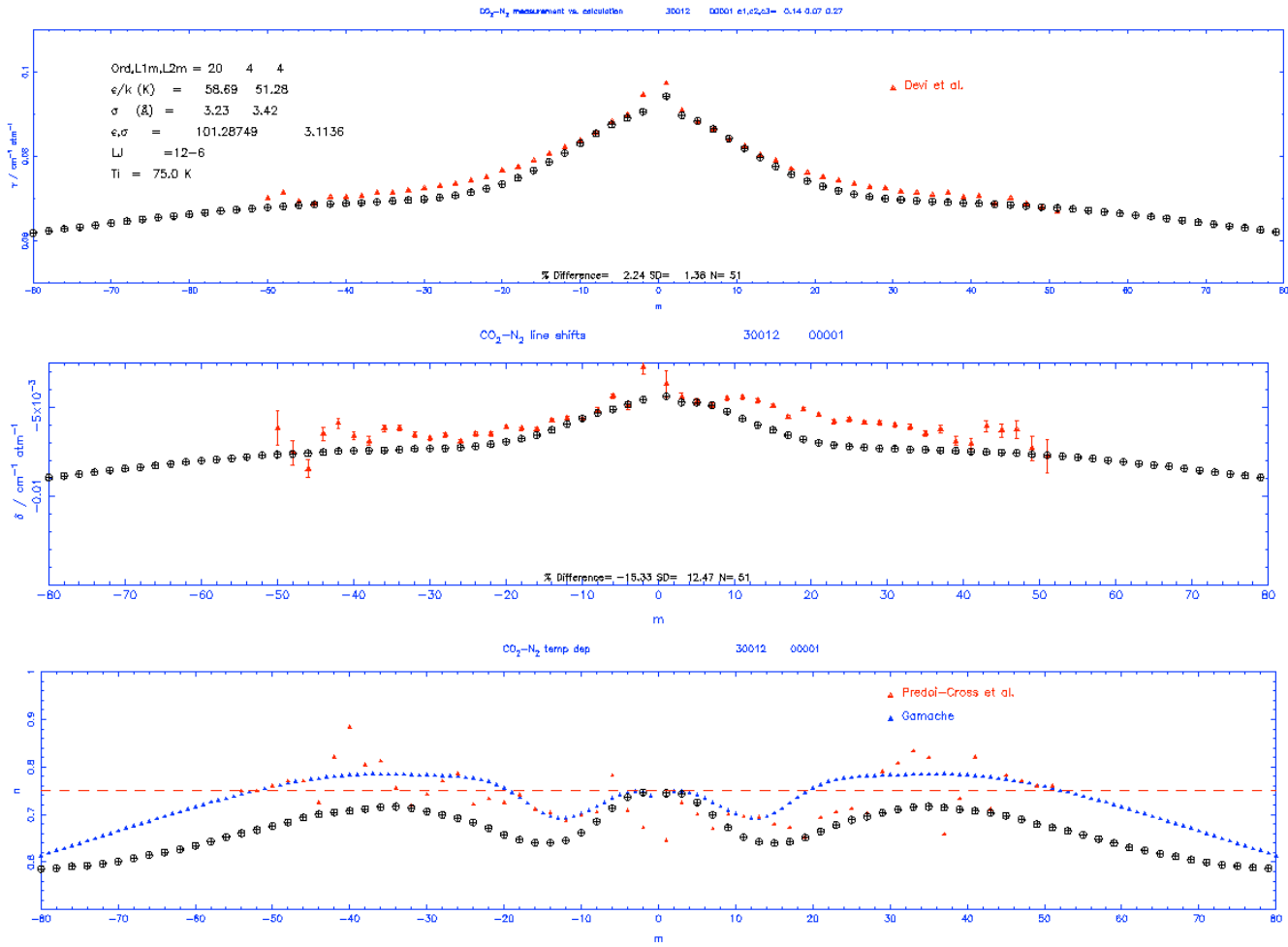
vibrational dependence of polarizability $0.263900\text{E}+010.140000\text{E}+000.700000\text{E}-010.268000\text{E}+00$



Pot a40 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 2.5% of $\sigma(\text{ON})$, Reduction of 32.6% of $\epsilon(\text{traj})$, Reduction of 29.3% of $\sigma(\text{traj})$

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

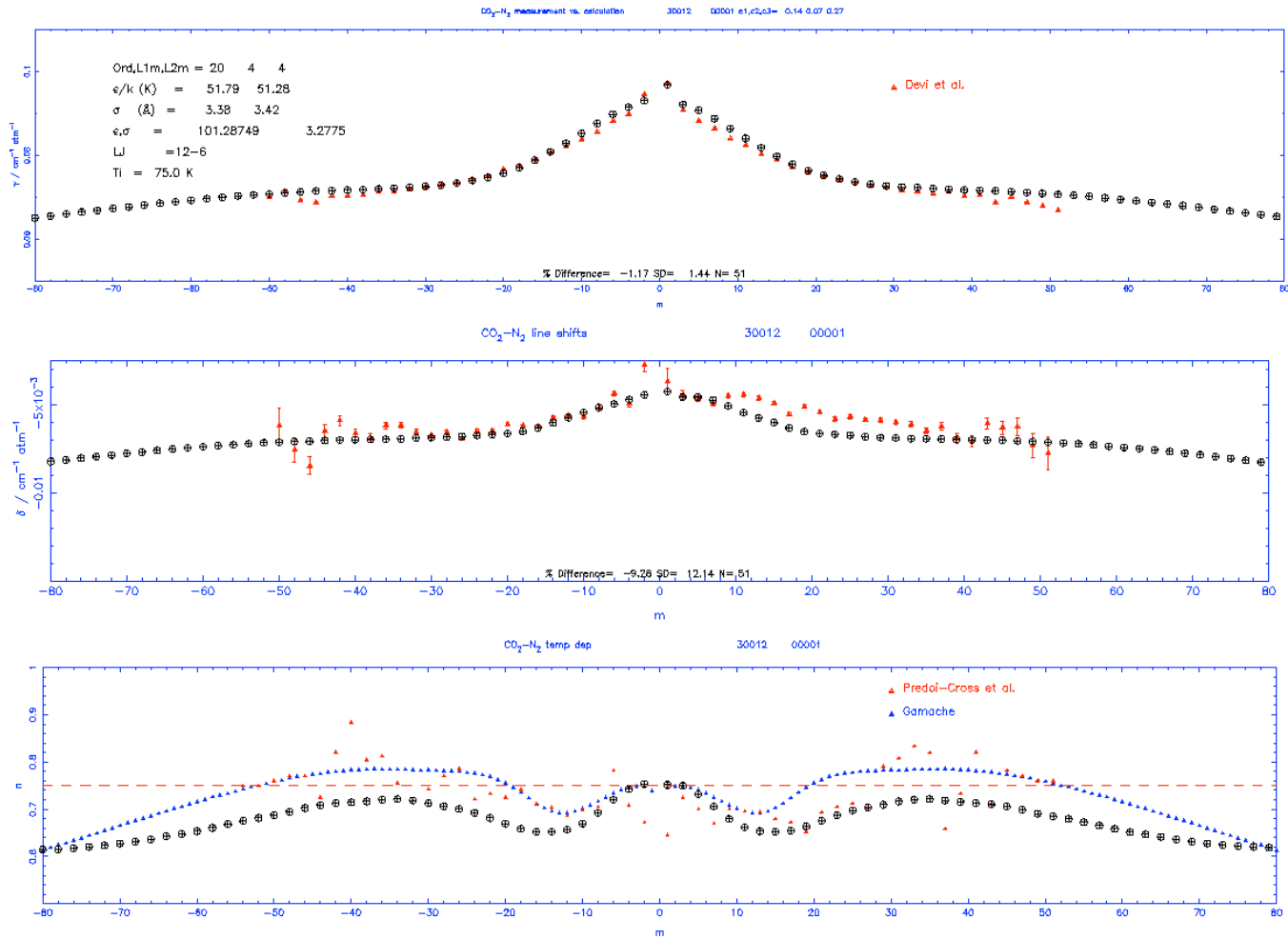
vibrational dependence of polarizability $0.263900\text{E}+010.140000\text{E}+000.700000\text{E}-010.268000\text{E}+00$



Pot a42 : (From Pot a00_1) Increase of 18% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 32.6% of $\epsilon(\text{traj})$, Reduction of 22.9% of $\sigma(\text{traj})$

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

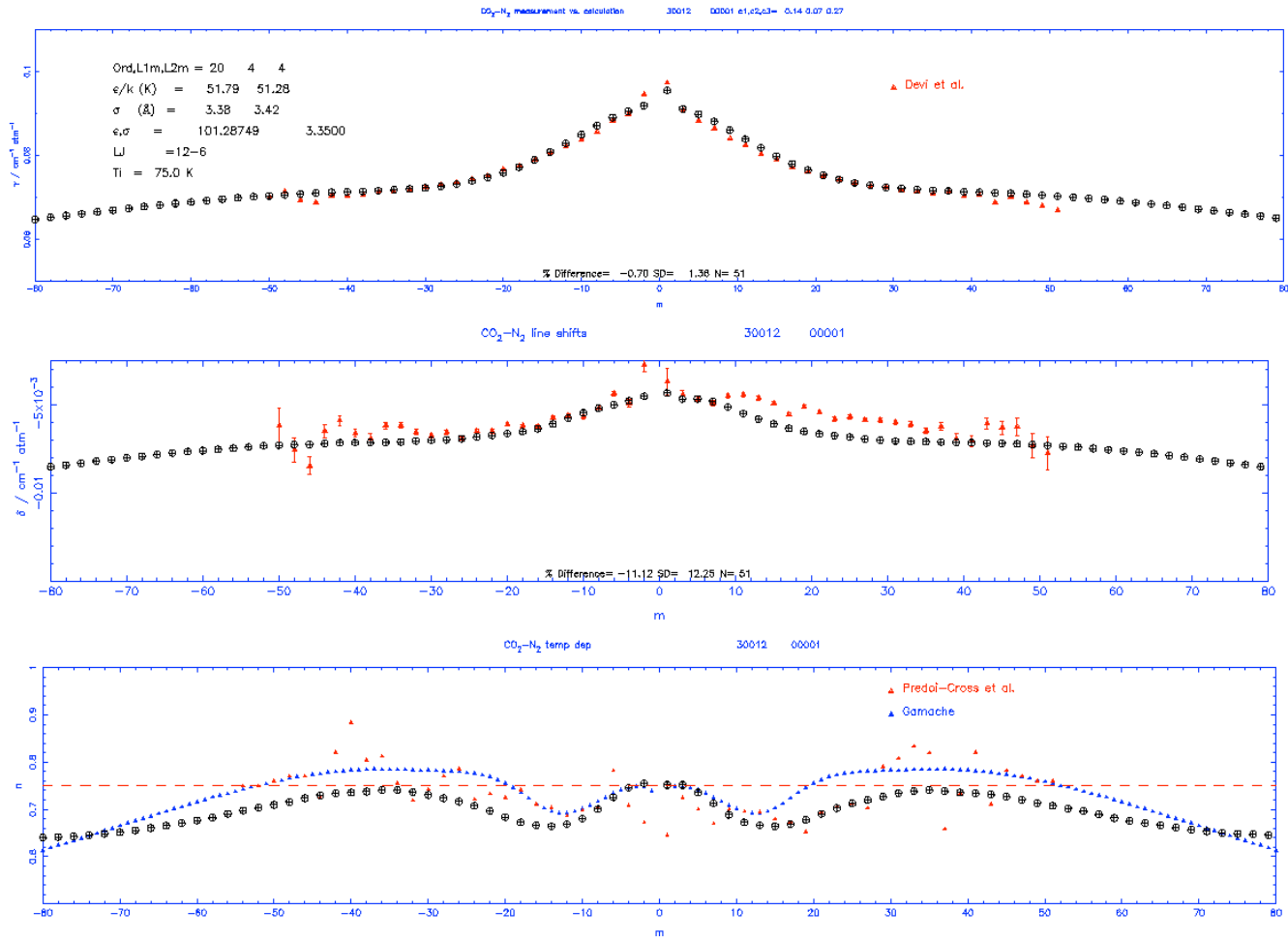
vibrational dependence of polarizability $0.263900\text{E}+010.140000\text{E}+000.700000\text{E}-010.268000\text{E}+00$



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

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

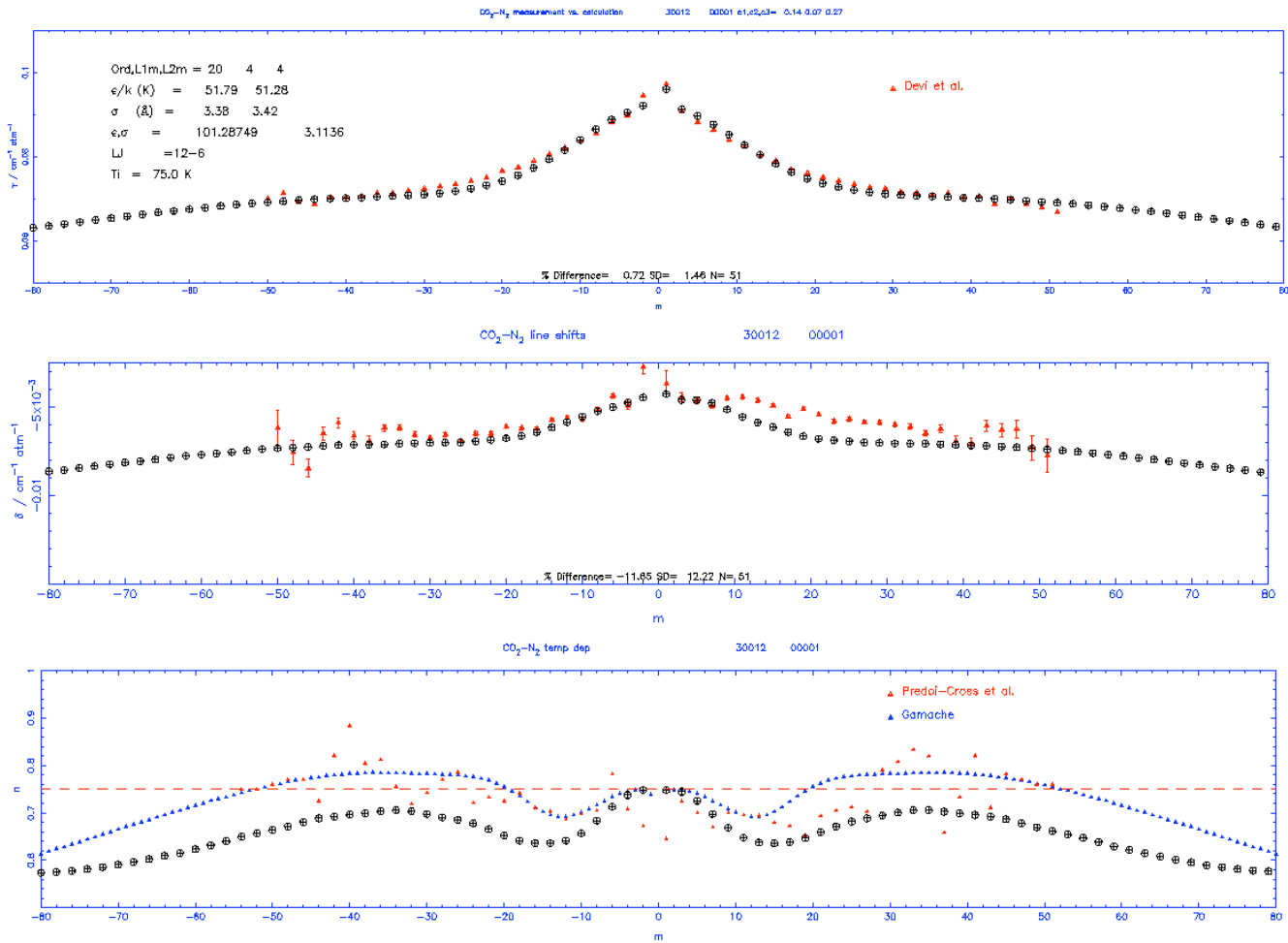
vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00



Pot a44 : (From Pot a00_1) Increase of 18% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 32.6% of $\epsilon(\text{traj})$, Reduction of 29.3% of $\sigma(\text{traj})$

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

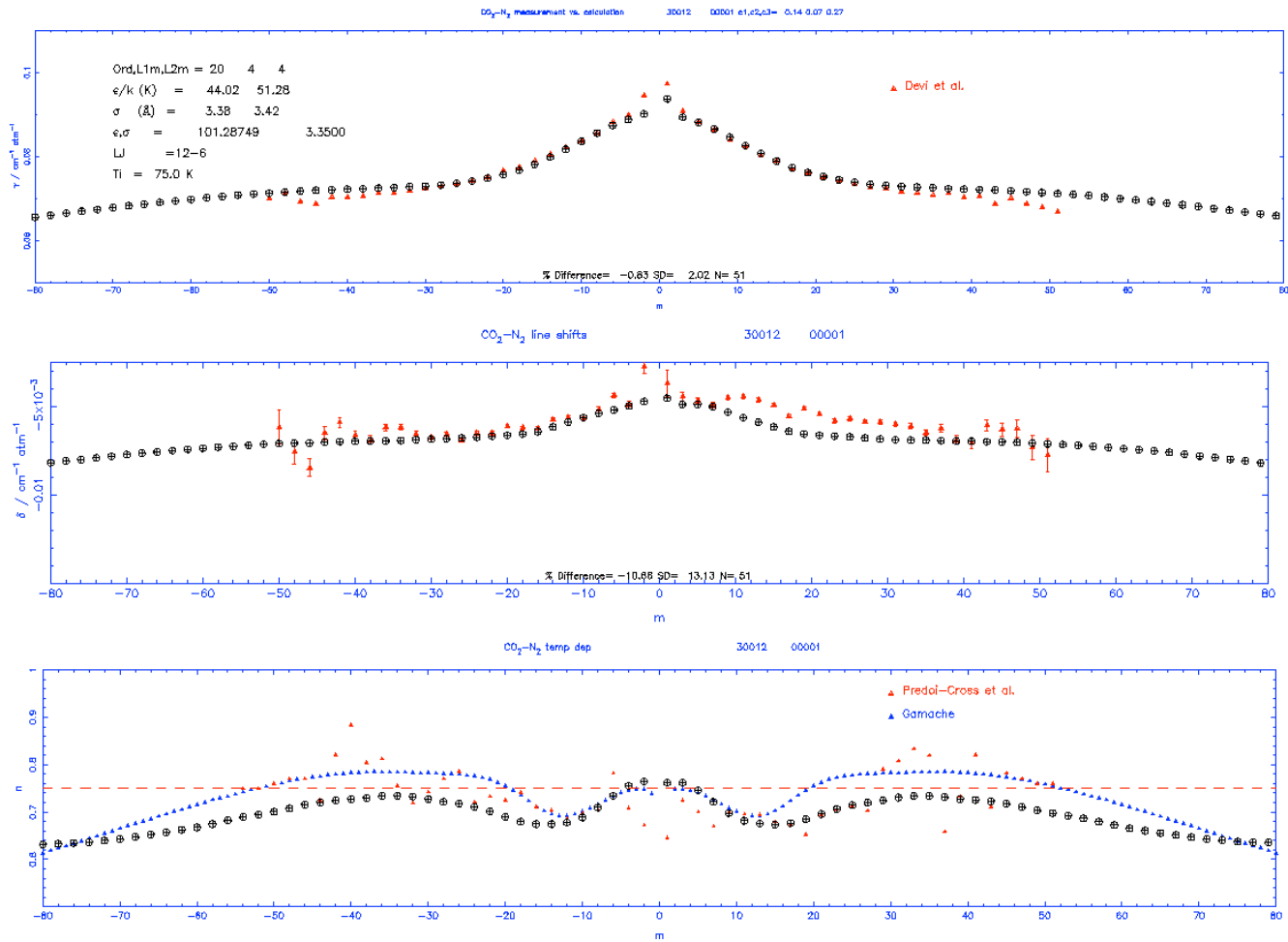
vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00



Pot a45 : (From Pot a00_1) Increase of 0.3% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 32.6% of $\epsilon(\text{traj})$, Reduction of 20.2% of $\sigma(\text{traj})$

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

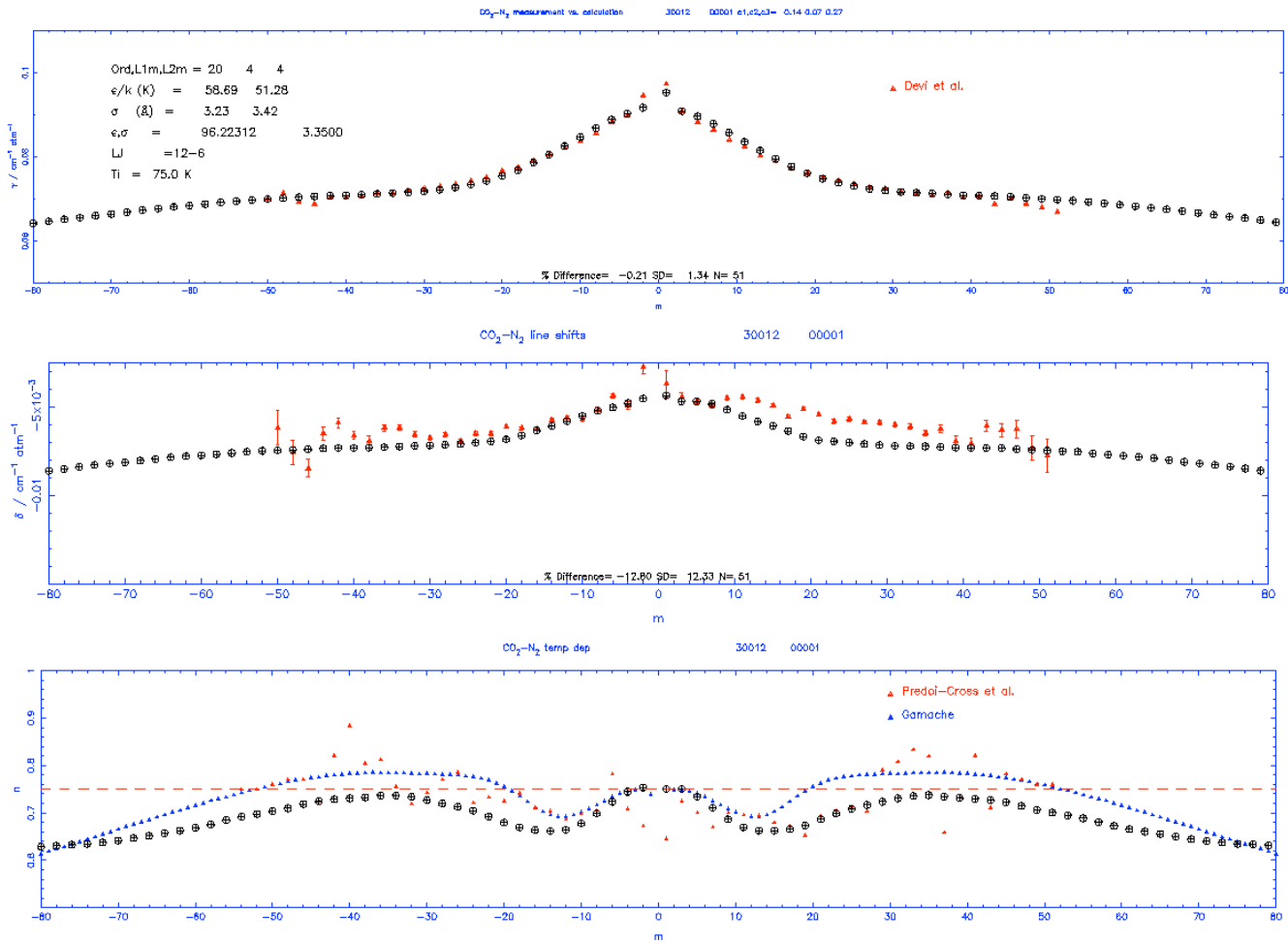
vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00



Pot a46 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 2.5% of $\sigma(\text{ON})$, Reduction of 39.6% of $\epsilon(\text{traj})$, Reduction of 20.2% of $\sigma(\text{traj})$

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

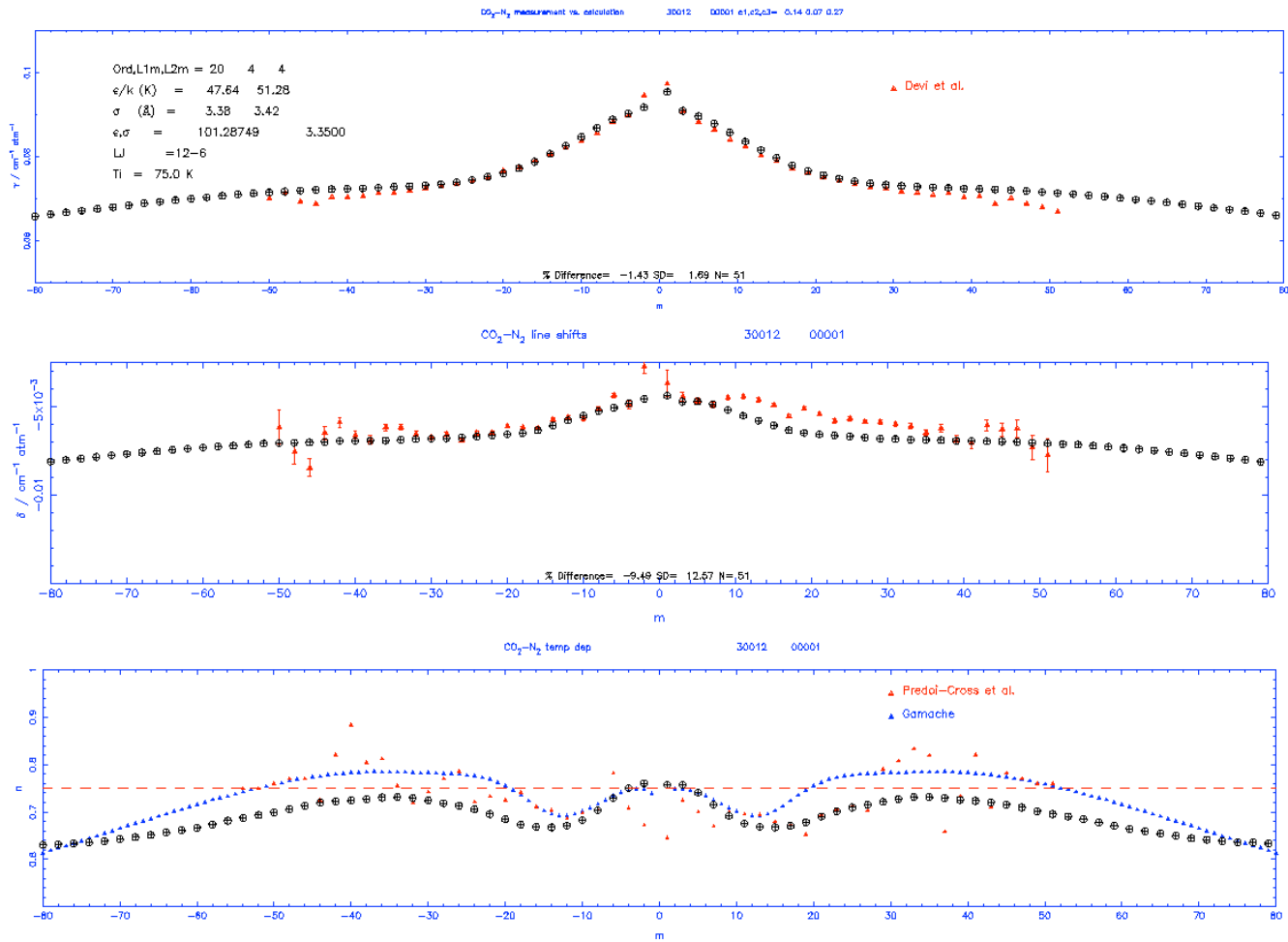
vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00



Pot a47 : (From Pot a00_1) Increase of 8.5% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 32.6% of $\epsilon(\text{traj})$, Reduction of 20.2% of $\sigma(\text{traj})$

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

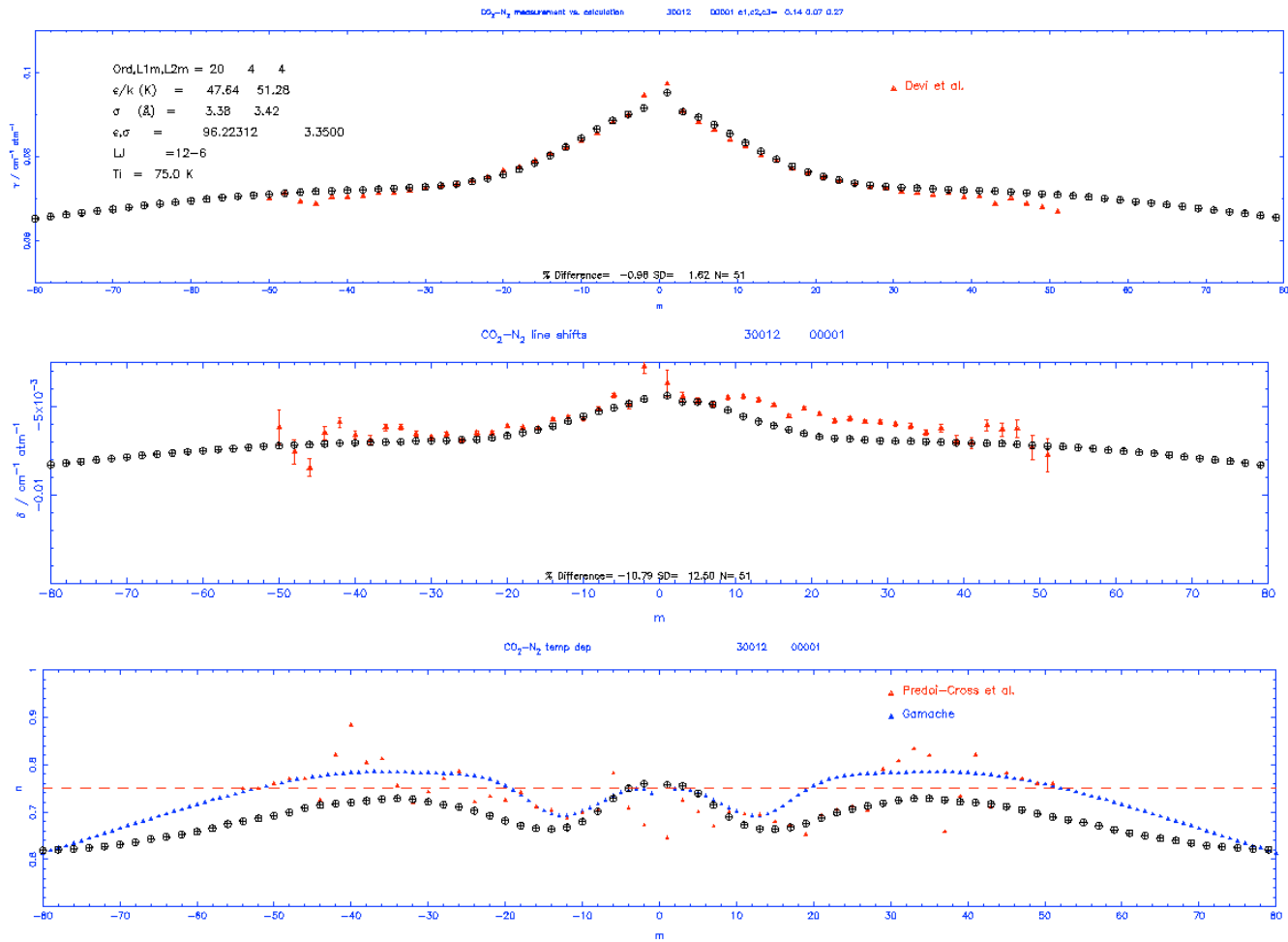
vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00



Pot a48 : (From Pot a00_1) Increase of 8.5% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 32.6% of $\epsilon(\text{traj})$, Reduction of 39.6% of $\sigma(\text{traj})$

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

vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00

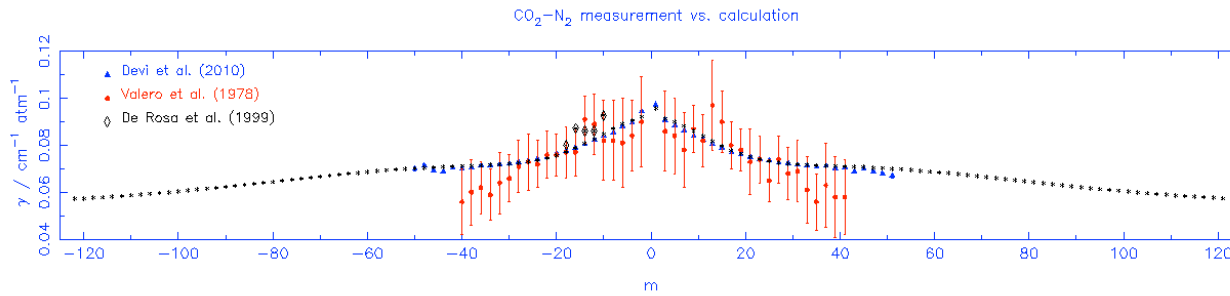


Pot a55 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 32.6% of $\epsilon(\text{traj})$, Reduction of 21.4% of $\sigma(\text{traj})$

$\epsilon(\text{ON})= 58.69$; $\sigma(\text{ON})=3.23$; $\epsilon(\text{traj})= 101.28749$; $\sigma(\text{traj})=3.31650$

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

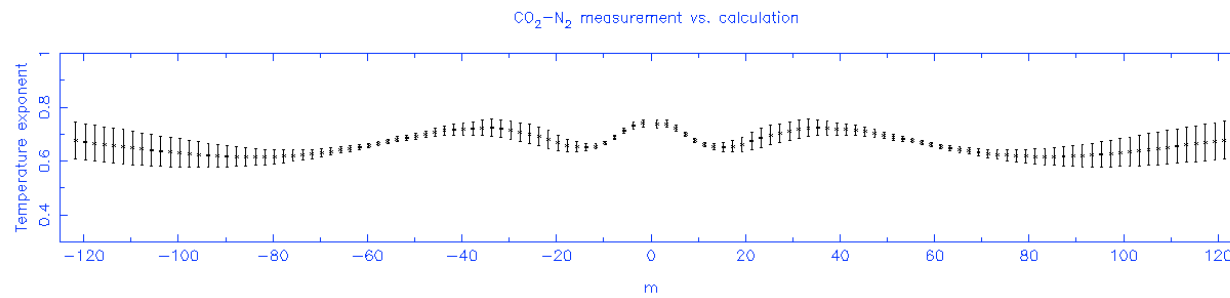
vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00



CO₂-N₂ measurement vs. calculation

$\delta / \text{cm}^{-1} \text{atm}^{-1} \times 10^{-3}$

m

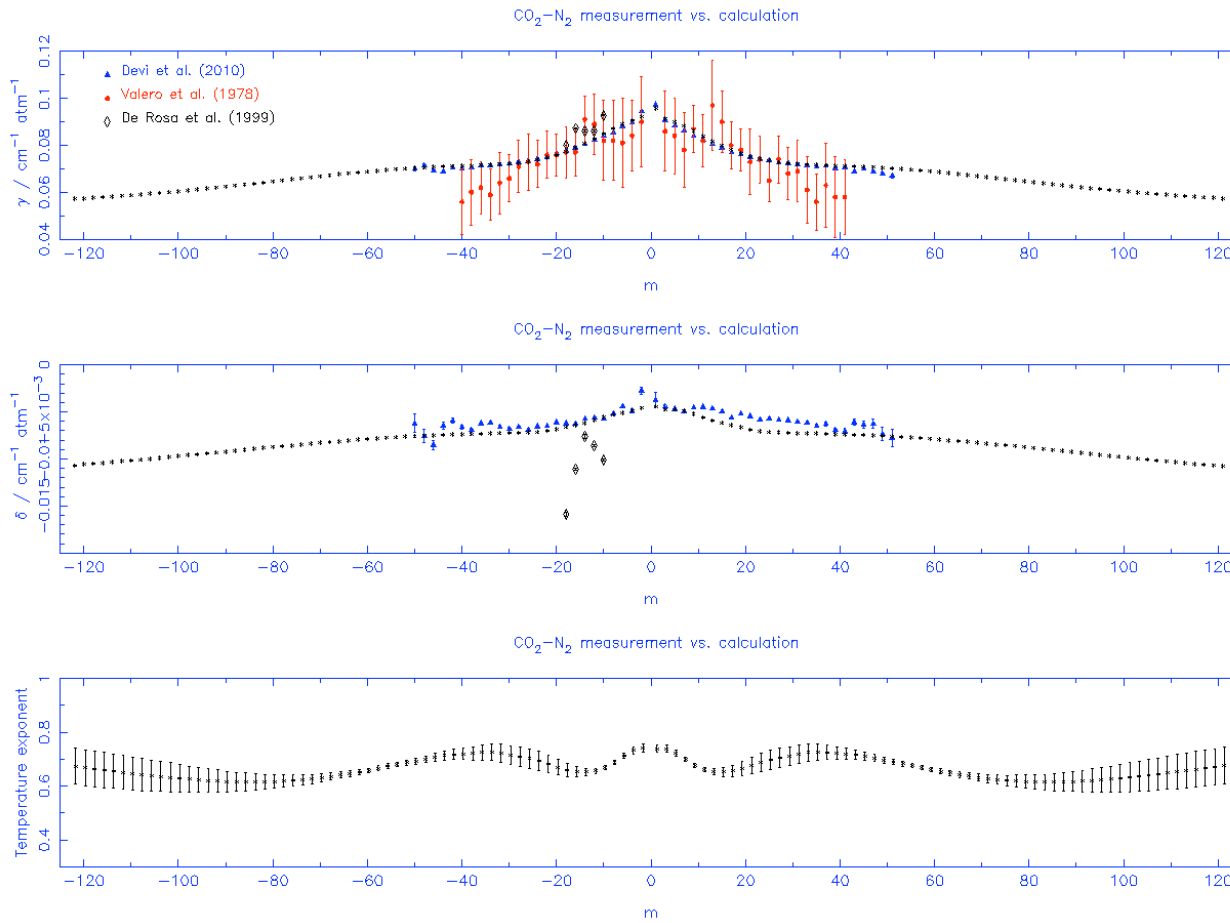


Pot a56 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 32.6% of $\epsilon(\text{traj})$, Reduction of 21.1% of $\sigma(\text{traj})$

$\epsilon(\text{ON})= 58.69$; $\sigma(\text{ON})=3.23$; $\epsilon(\text{traj})= 101.28749$; $\sigma(\text{traj})=3.32655$

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

vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00

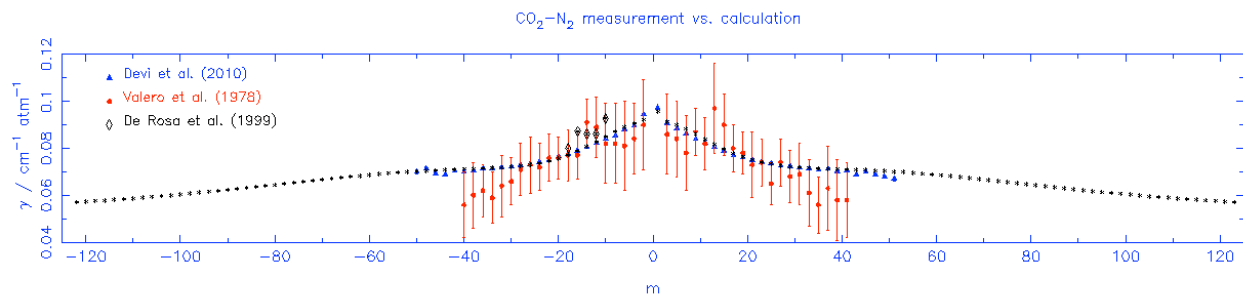


Pot a57 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 39.6% of $\epsilon(\text{traj})$, Reduction of 20.2% of $\sigma(\text{traj})$

$\epsilon(\text{ON})= 58.69$; $\sigma(\text{ON})=3.23$; $\epsilon(\text{traj})= 96.22312$; $\sigma(\text{traj})=3.35000$

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

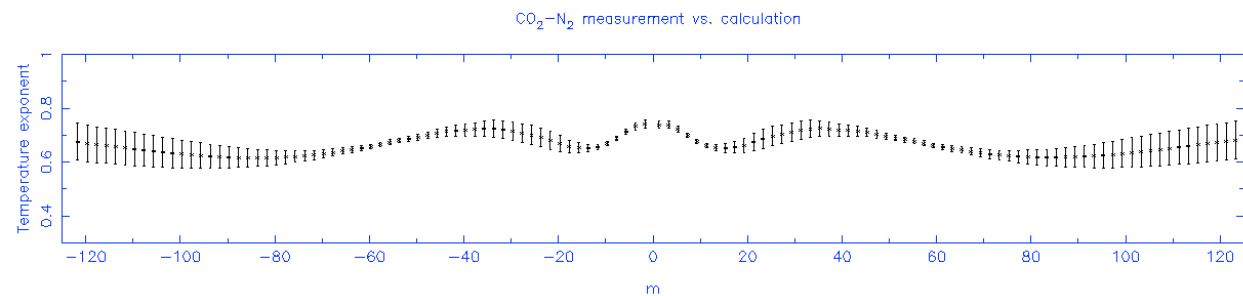
vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00



CO₂-N₂ measurement vs. calculation

$\delta / \text{cm}^{-1} \text{atm}^{-1} \times 10^{-3}$

m

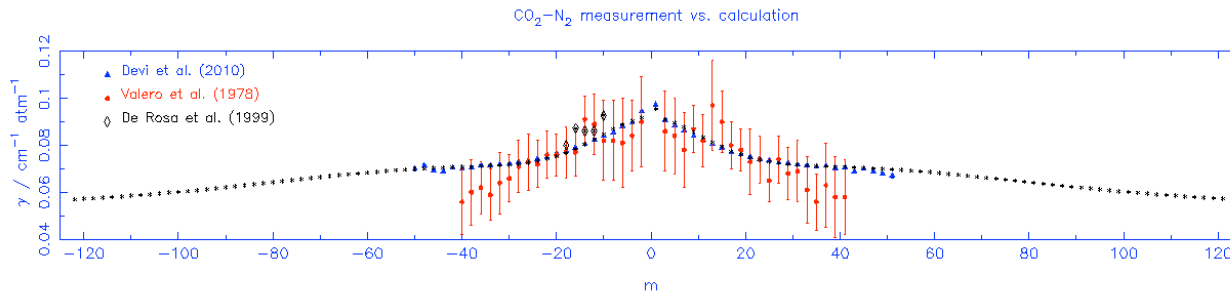


Pot a58 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 31.3% of $\epsilon(\text{traj})$, Reduction of 22.9% of $\sigma(\text{traj})$

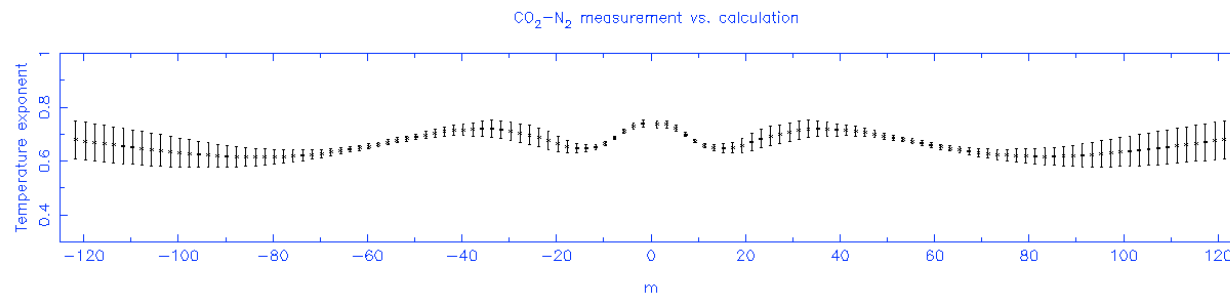
$\epsilon(\text{ON})= 58.69$; $\sigma(\text{ON})=3.23$; $\epsilon(\text{traj})= 102.30036$; $\sigma(\text{traj})= 3.27750$

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

vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00



CO₂-N₂ measurement vs. calculation

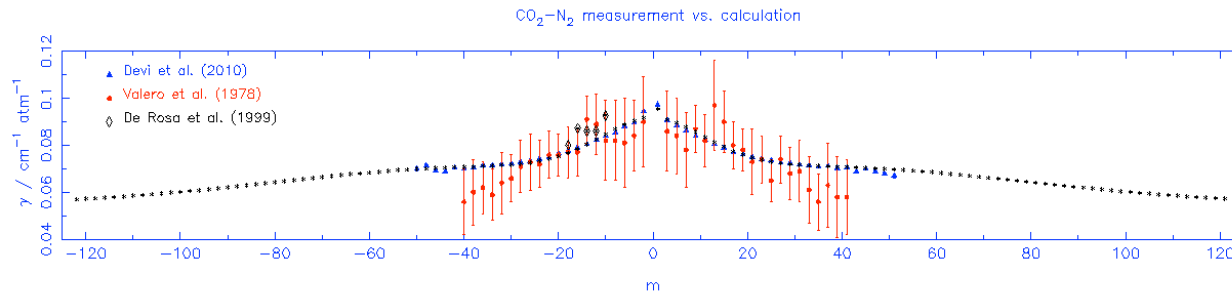


Pot a59 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 31% of $\epsilon(\text{traj})$, Reduction of 22.9% of $\sigma(\text{traj})$

$\epsilon(\text{ON})= 58.69$; $\sigma(\text{ON})=3.23$; $\epsilon(\text{traj})= 102.50294$; $\sigma(\text{traj})= 3.27750$

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

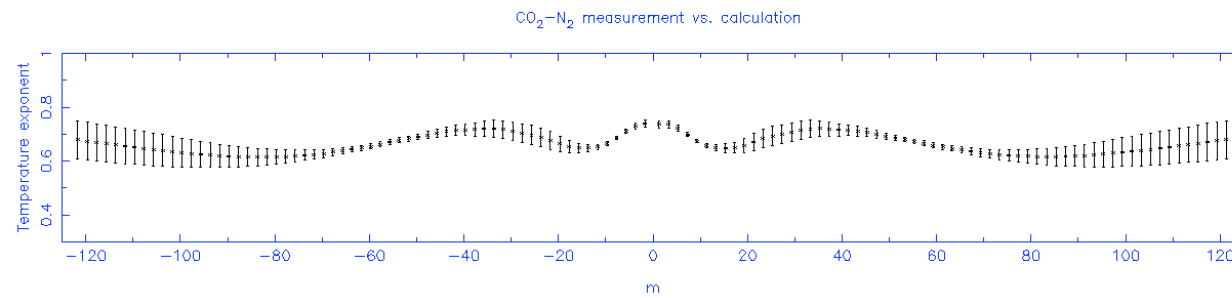
vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00



CO₂-N₂ measurement vs. calculation

$\delta / \text{cm}^{-1} \text{atm}^{-1}$

m

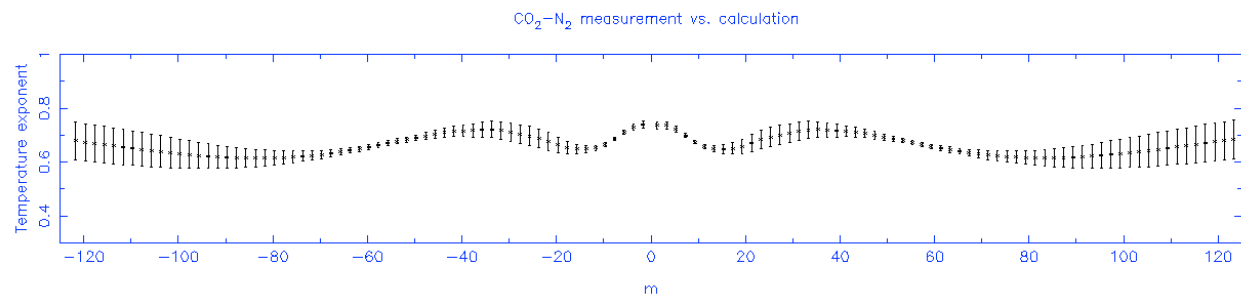
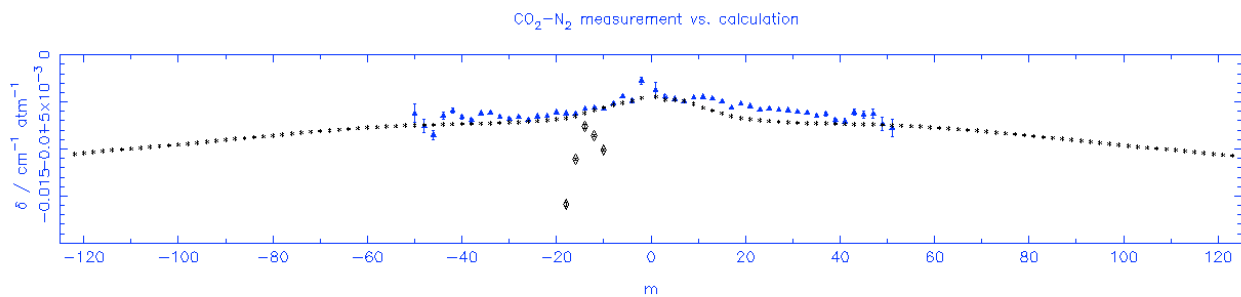
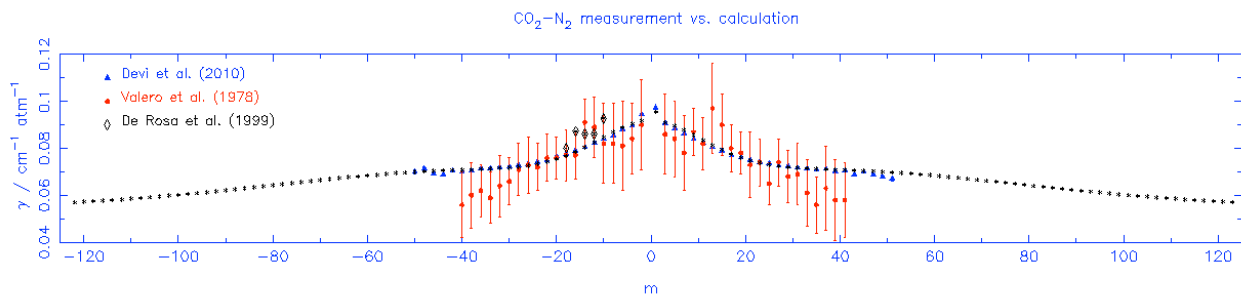


Pot a60 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 30.7% of $\epsilon(\text{traj})$, Reduction of 22.9% of $\sigma(\text{traj})$

$\epsilon(\text{ON})= 58.69$; $\sigma(\text{ON})=3.23$; $\epsilon(\text{traj})= 102.80680$; $\sigma(\text{traj})= 3.27750$

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

vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00

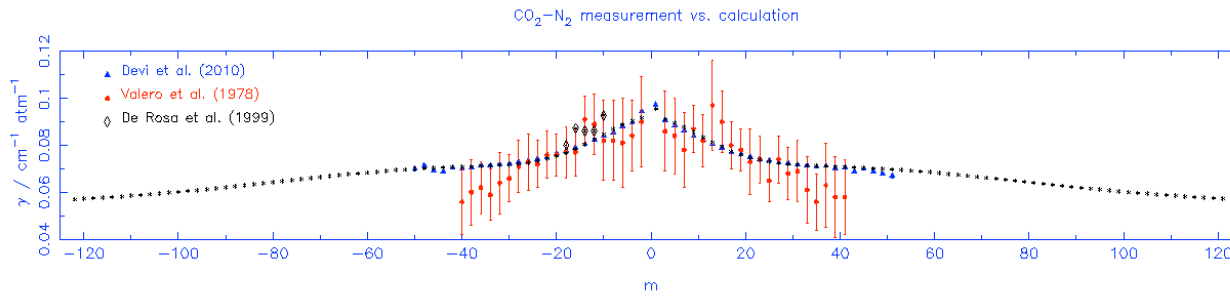


Pot a61 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 30.8% of $\epsilon(\text{traj})$, Reduction of 22.9% of $\sigma(\text{traj})$

$\epsilon(\text{ON})= 58.69$; $\sigma(\text{ON})=3.23$; $\epsilon(\text{traj})= 102.65487$; $\sigma(\text{traj})= 3.27750$

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

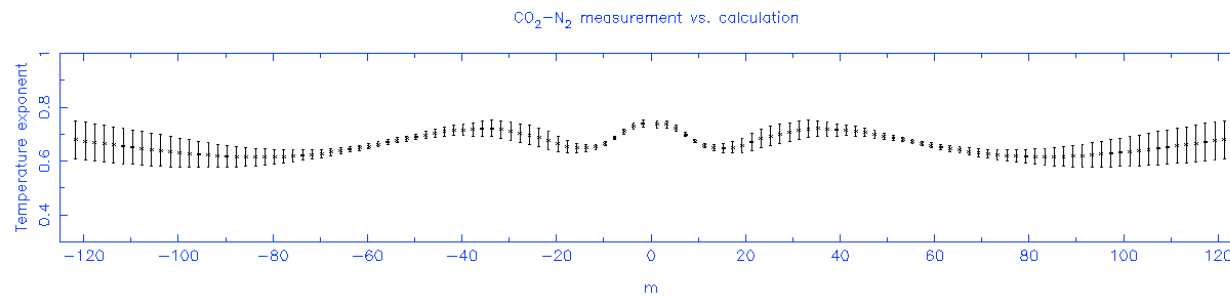
vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00



CO₂-N₂ measurement vs. calculation

$\delta / \text{cm}^{-1} \text{atm}^{-1}$

m

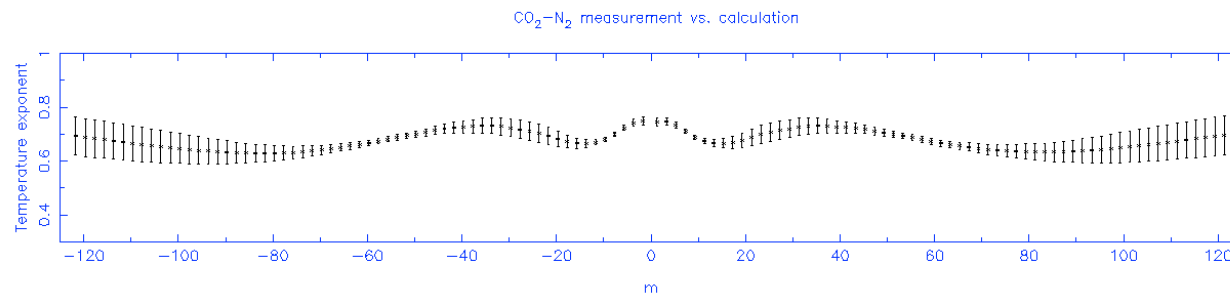
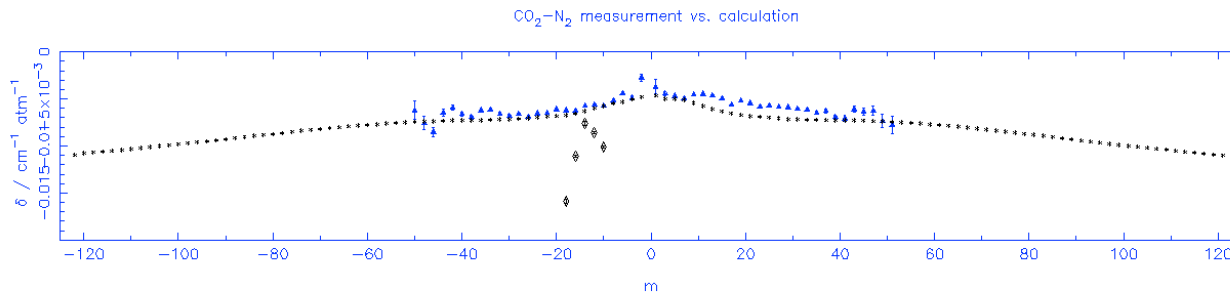
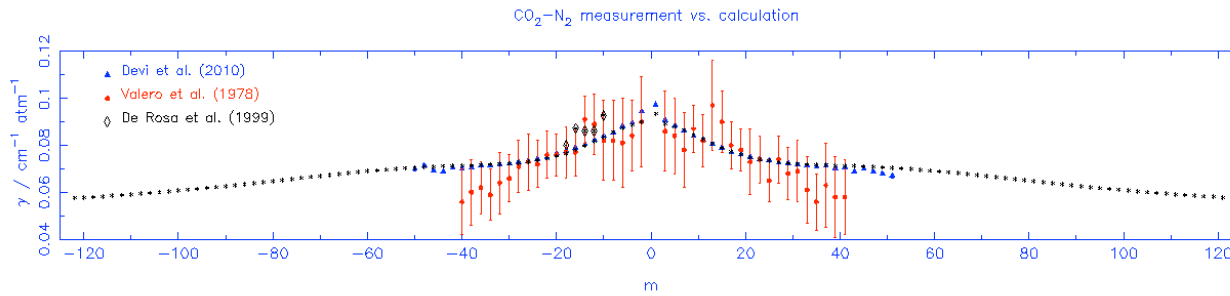


Pot a62 : (From Pot a00_1) Increase of 18% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 32.6% of $\epsilon(\text{traj})$, Reduction of 20.2% of $\sigma(\text{traj})$

$\epsilon(\text{ON})= 51.79$; $\sigma(\text{ON})=3.23$; $\epsilon(\text{traj})= 101.28749$; $\sigma(\text{traj})= 3.35000$

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

vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00

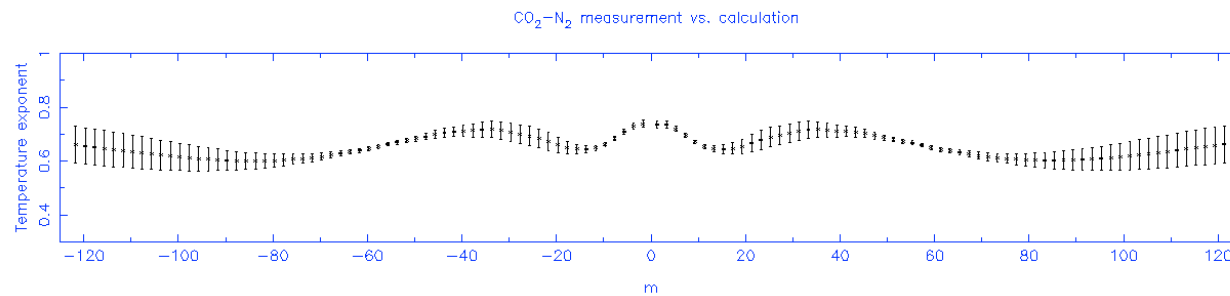
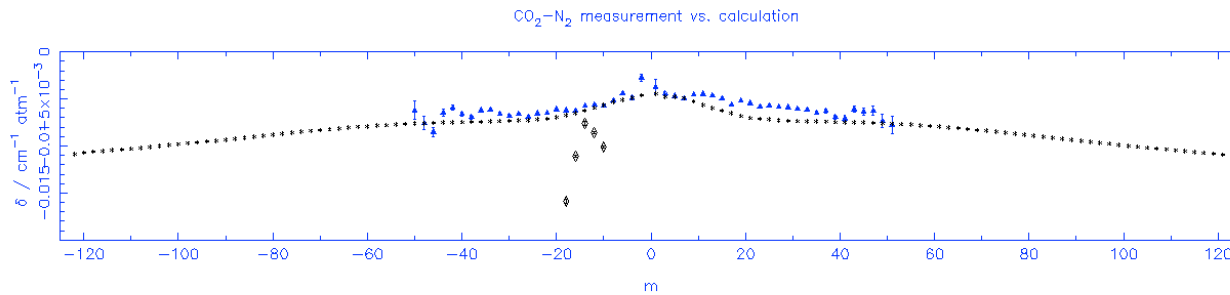
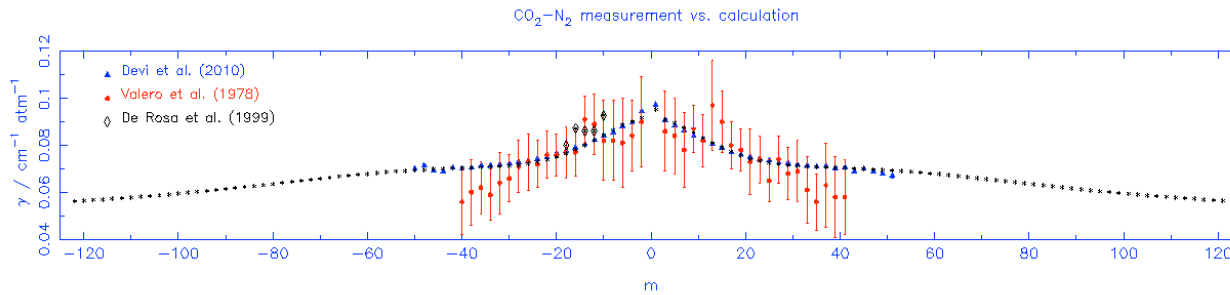


Pot a63 : (From Pot a00_1) Increase of 33.9% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 39.6% of $\epsilon(\text{traj})$, Reduction of 22.9% of $\sigma(\text{traj})$

$\epsilon(\text{ON})= 58.79$; $\sigma(\text{ON})=3.23$; $\epsilon(\text{traj})= 96.22311$; $\sigma(\text{traj})= 3.27750$

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

vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00

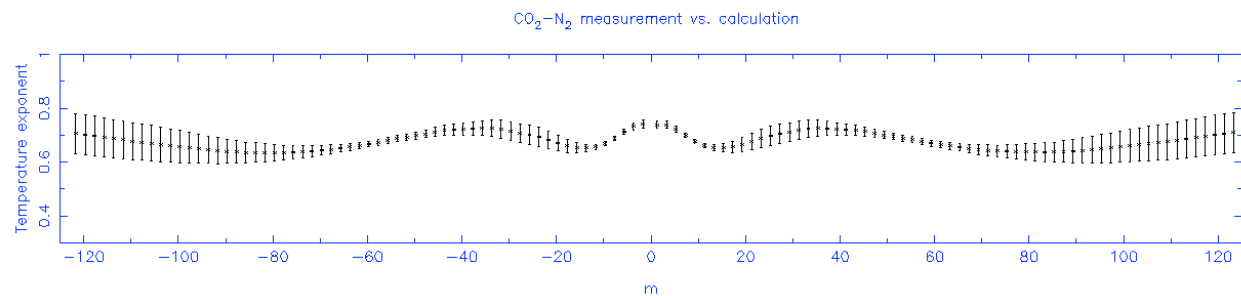
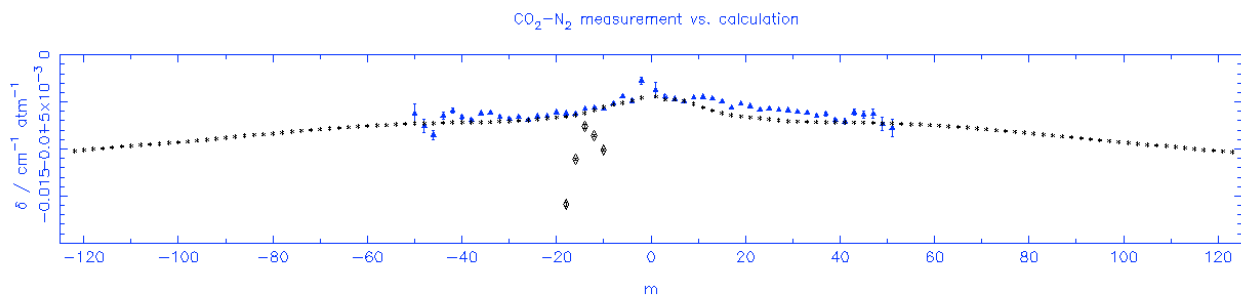
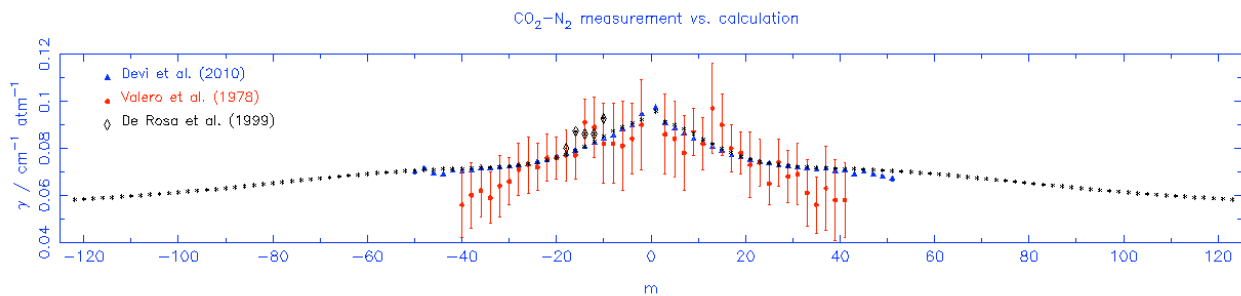


Pot a64 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 20.6% of $\epsilon(\text{traj})$, Reduction of 22.9% of $\sigma(\text{traj})$

$\epsilon(\text{ON})= 58.69$; $\sigma(\text{ON})=3.23$; $\epsilon(\text{traj})= 111.41624$; $\sigma(\text{traj})= 3.27750$

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

vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00

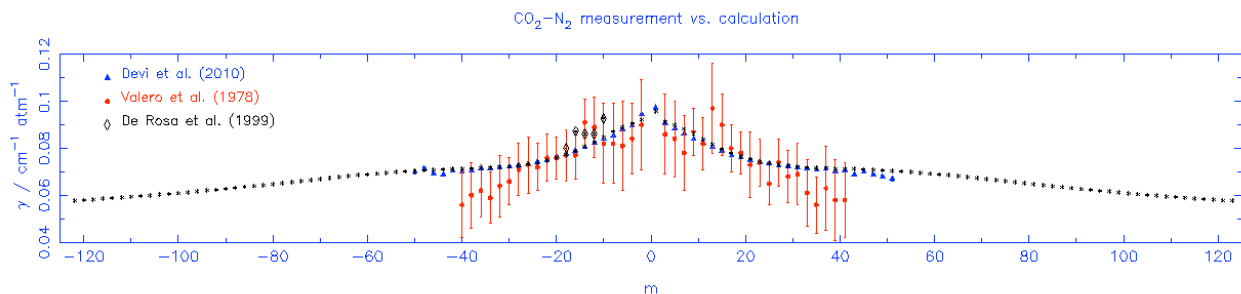


Pot a65 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 9.5% of $\epsilon(\text{traj})$, Reduction of 25.6% of $\sigma(\text{traj})$

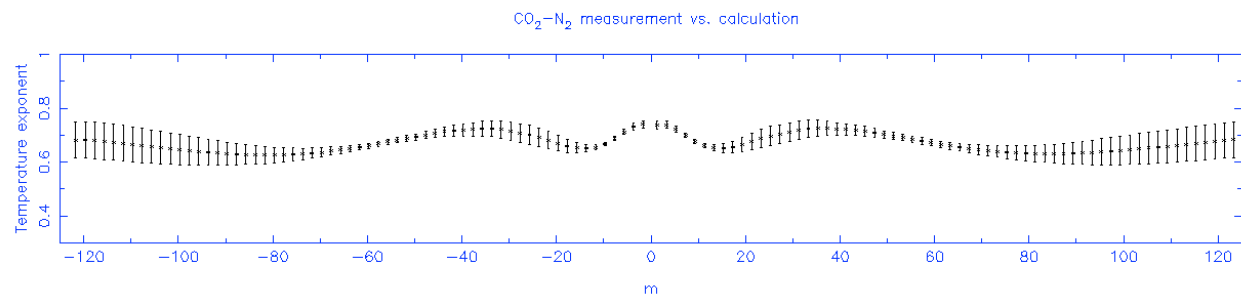
$\epsilon(\text{ON})= 58.69$; $\sigma(\text{ON})=3.23$; $\epsilon(\text{traj})= 122.55786$; $\sigma(\text{traj})= 3.20657$

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

vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00



CO₂-N₂ measurement vs. calculation

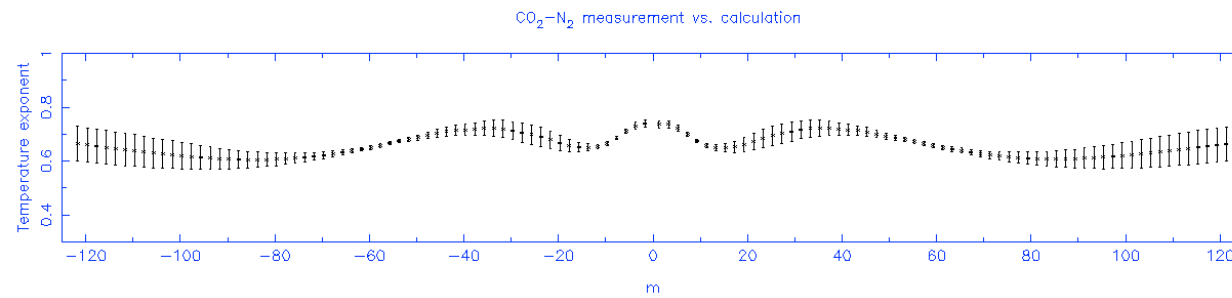
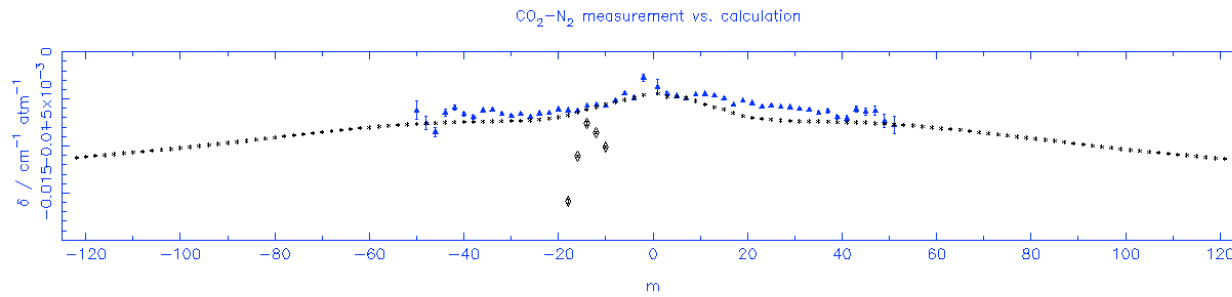
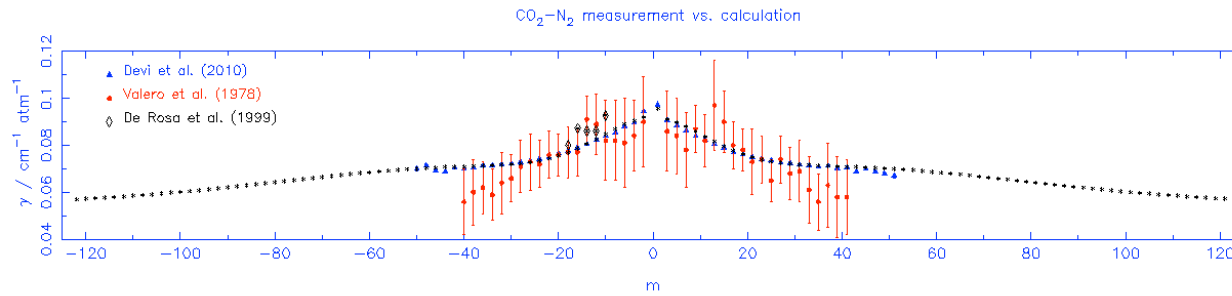


Pot a66 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Increase of 0.4% of $\epsilon(\text{traj})$, Reduction of 28.4% of $\sigma(\text{traj})$

$\epsilon(\text{ON})= 58.69$; $\sigma(\text{ON})=3.23$; $\epsilon(\text{traj})= 134.81365$; $\sigma(\text{traj})= 3.13717$

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

vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00

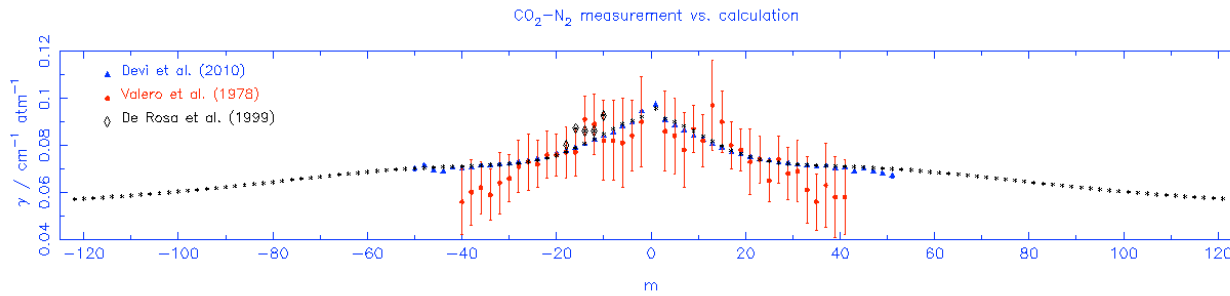


Pot a67 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 24.8% of $\epsilon(\text{traj})$, Reduction of 22.9% of $\sigma(\text{traj})$

$\epsilon(\text{ON})= 58.69$; $\sigma(\text{ON})=3.23$; $\epsilon(\text{traj})= 107.61796$; $\sigma(\text{traj})= 3.27750$

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

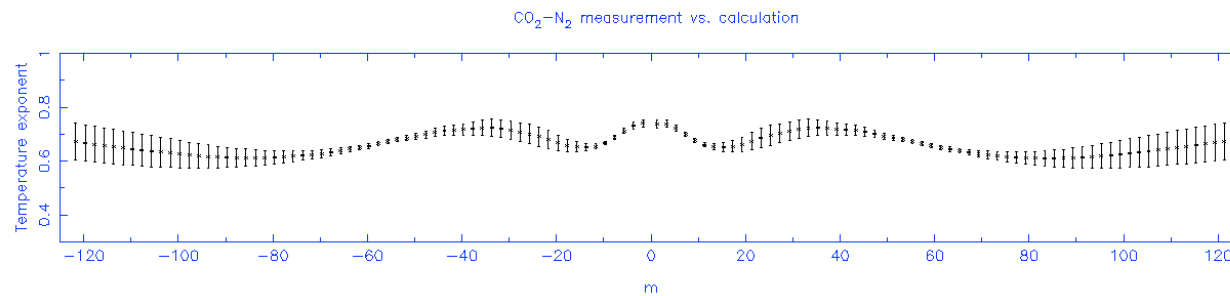
vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00



CO₂-N₂ measurement vs. calculation

$\delta / \text{cm}^{-1} \text{atm}^{-1}$

m

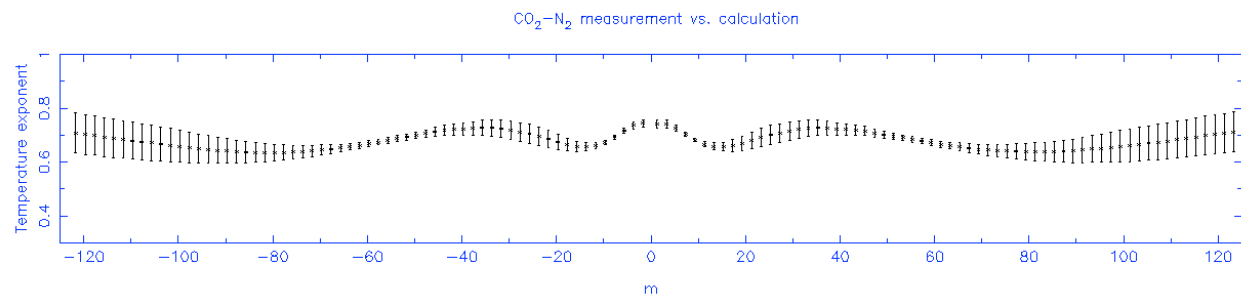
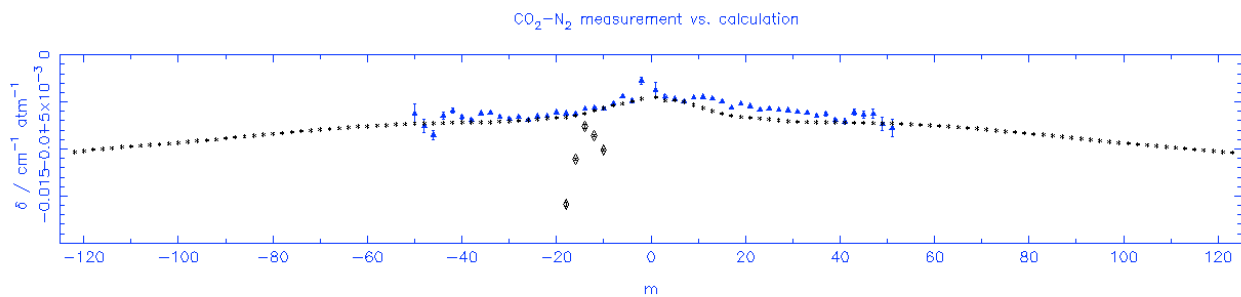
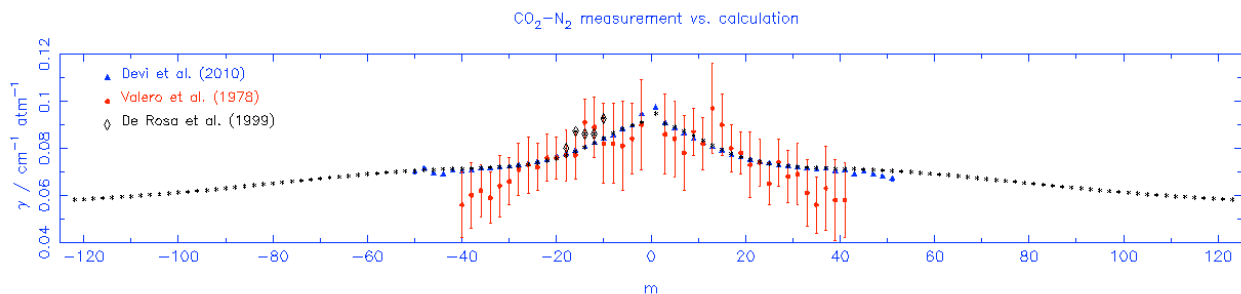


Pot a68 : (From Pot a00_1) Increase of 27% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 20.6% of $\epsilon(\text{traj})$, Reduction of 22.9% of $\sigma(\text{traj})$

$\epsilon(\text{ON})= 55.76$; $\sigma(\text{ON})=3.23$; $\epsilon(\text{traj})= 111.41624$; $\sigma(\text{traj})= 3.27750$

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

vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00

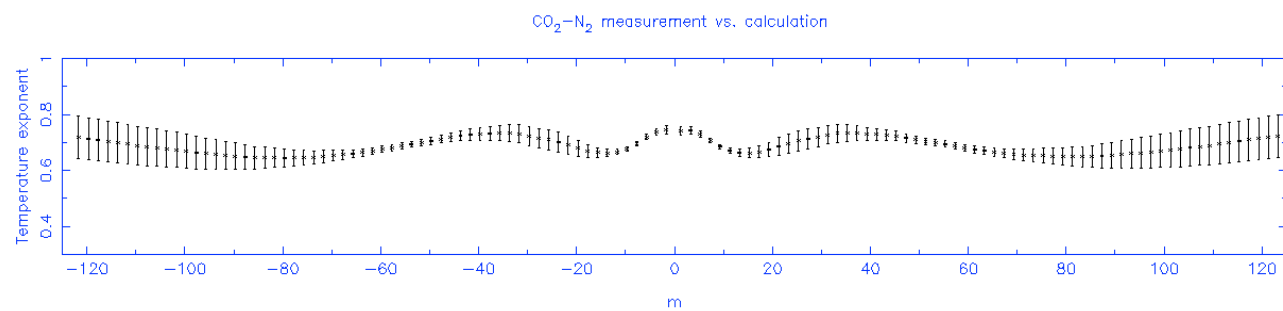
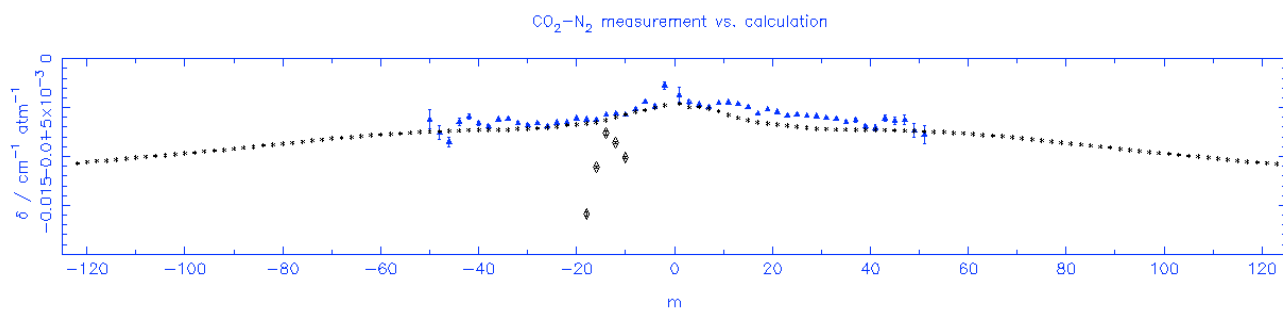
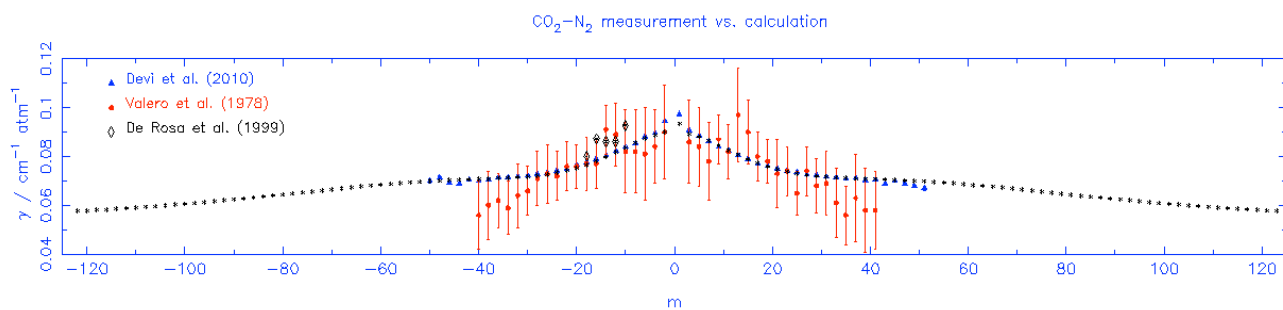


Pot a69 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Reduction of 20.6% of $\epsilon(\text{traj})$, Reduction of 22.9% of $\sigma(\text{traj})$

$\epsilon(\text{ON})= 58.69$; $\sigma(\text{ON})=3.15$; $\epsilon(\text{traj})= 111.41624$; $\sigma(\text{traj})= 3.27750$

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

vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00

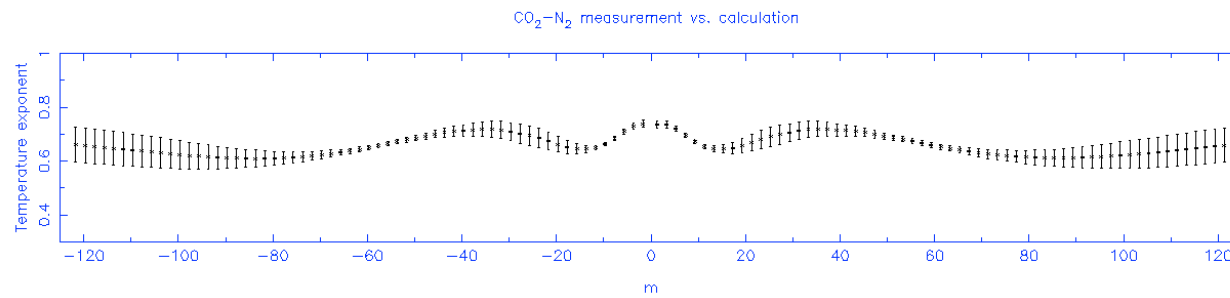
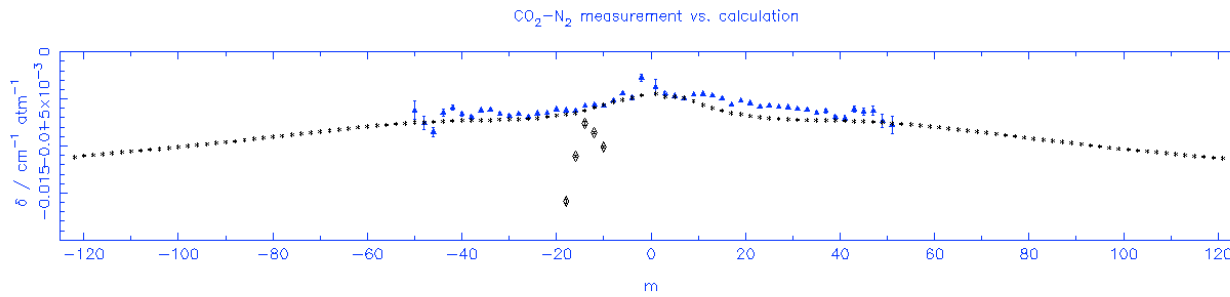
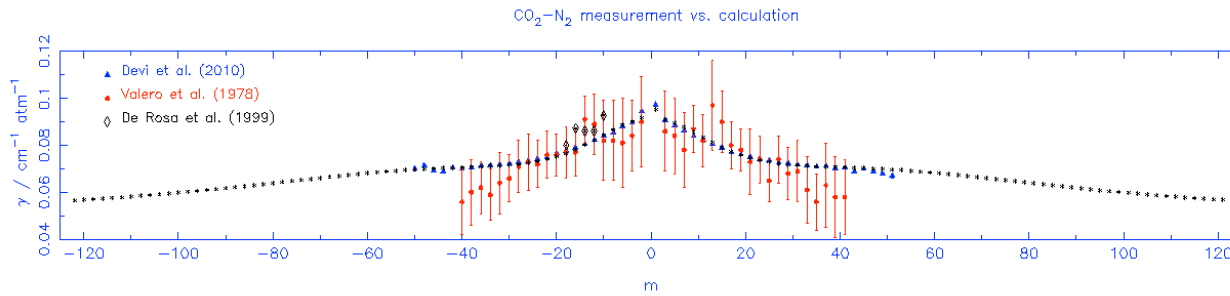


Pot a70 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 7.3% of $\sigma(\text{ON})$, Reduction of 20.6% of $\epsilon(\text{traj})$, Reduction of 25.6% of $\sigma(\text{traj})$

$\epsilon(\text{ON})= 58.69$; $\sigma(\text{ON})=3.23$; $\epsilon(\text{traj})= 111.41624$; $\sigma(\text{traj})= 3.20657$

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

vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00

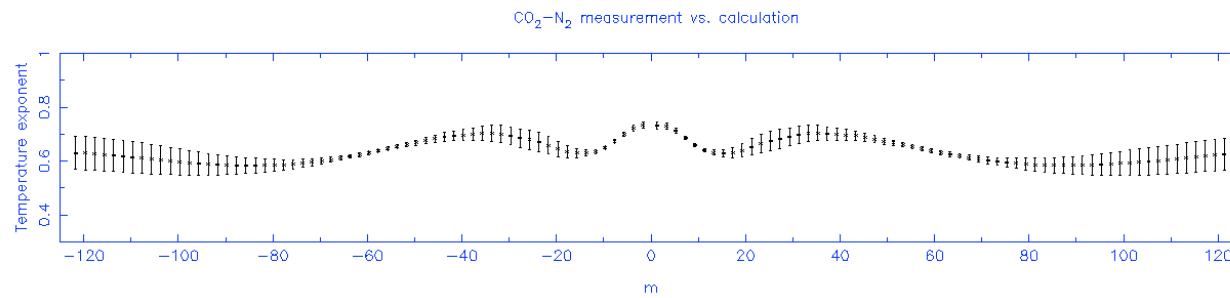
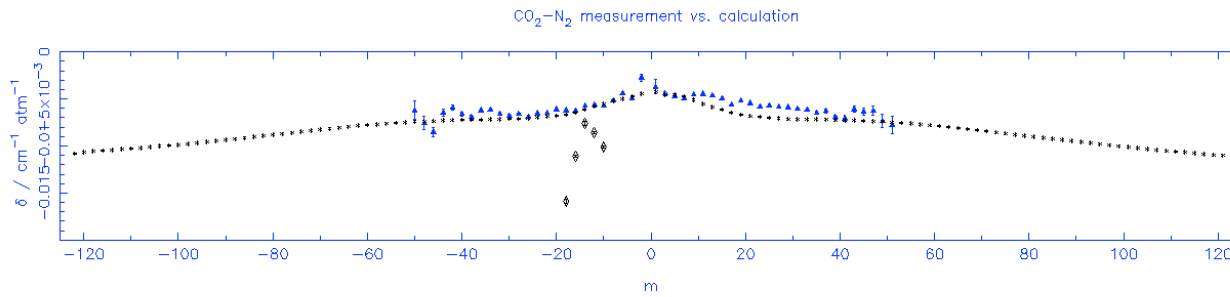
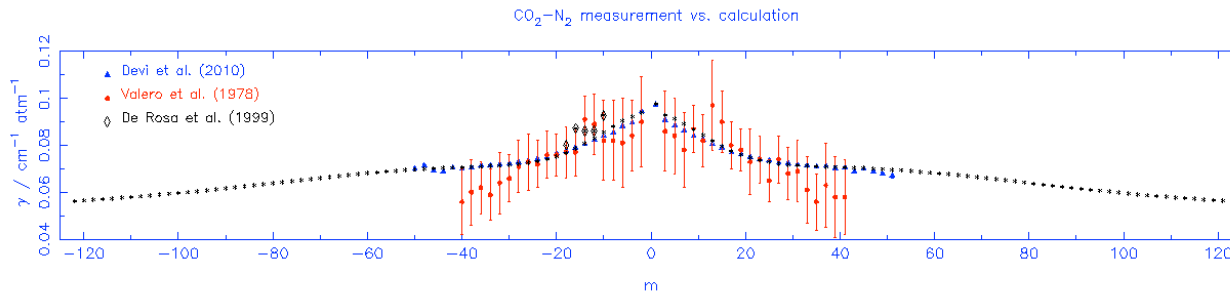


Pot a71 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 5.1% of $\sigma(\text{ON})$, Reduction of 20.6% of $\epsilon(\text{traj})$, Reduction of 28.4% of $\sigma(\text{traj})$

$\epsilon(\text{ON})= 58.69$; $\sigma(\text{ON})=3.31$; $\epsilon(\text{traj})= 111.41624$; $\sigma(\text{traj})= 3.13717$

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

vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00

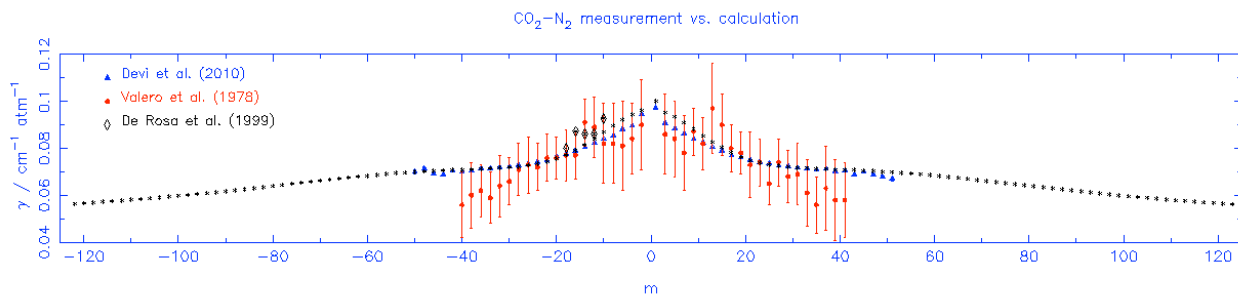


Pot a72 : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 7.9% of $\sigma(\text{ON})$, Reduction of 20.6% of $\epsilon(\text{traj})$, Reduction of 31.2% of $\sigma(\text{traj})$

$\epsilon(\text{ON})= 58.69$; $\sigma(\text{ON})=3.40$; $\epsilon(\text{traj})= 111.41624$; $\sigma(\text{traj})= 3.06928$

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

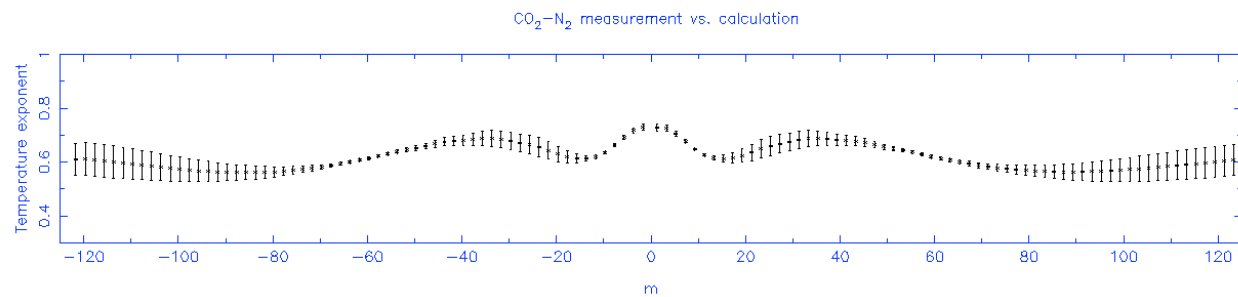
vibrational dependence of polarizability 0.263900E+01 0.140000E+00 0.700000E-01 0.268000E+00



CO₂-N₂ measurement vs. calculation

$\delta / \text{cm}^{-1} \text{atm}^{-1}$

m



Pot a39 –Figure 6 of publication : (From Pot a00_1) Increase of 33.7% of $\epsilon(\text{ON})$, Increase of 2.5% of $\sigma(\text{ON})$, Reduction of 24.6% of $\epsilon(\text{traj})$, Reduction of 18.6% of $\sigma(\text{traj})$

$\epsilon(\text{ON})= 58.69$; $\sigma(\text{ON})=3.23$; $\epsilon(\text{traj})= 101.29$; $\sigma(\text{traj})= 3.2775$

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

vibrational dependence of polarizability $0.263900\text{E}+01$ $0.140000\text{E}+00$ $0.700000\text{E}-01$ $0.268000\text{E}+00$

