

r²SCAN-3c(STO): Efficient, Robust & Reliable composite DFT method in ADF



OVERVIEW

1. Introduction to the “3c”-family
2. r^2 SCAN-3c(STO)
3. Results
4. Conclusion
5. Demo

1. INTRODUCTION TO THE “3c” FAMILY

1. INTRODUCTION TO THE “3c” FAMILY

	HF-3c	PBEh-3c	B97-3c	$r^2\text{SCAN-3c}$
AO Basis Set	Minimal	mSVP	mTZVP	mTZVPP/mTZ2P
No. of parameters in F_{xc}	0	3	10	Unaltered
Fock exchange (%)	100	42	0	0
Dispersion	D3	D3	D3	D4
SRB correction	✓	X	✓	X
BSSE correction (gCP)	✓	✓	X	✓

“3c” = 3 corrections

2. r^2 SCAN-3c(STO)

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Density
Functional
 r^2 SCAN

Basis Set
mTZ2P

Dispersion
Correction

BSSE
Correction

2. $r^2\text{SCAN-3c(STO)}$

Density
Functional
 $r^2\text{SCAN}$

Basis Set
mTZ2P

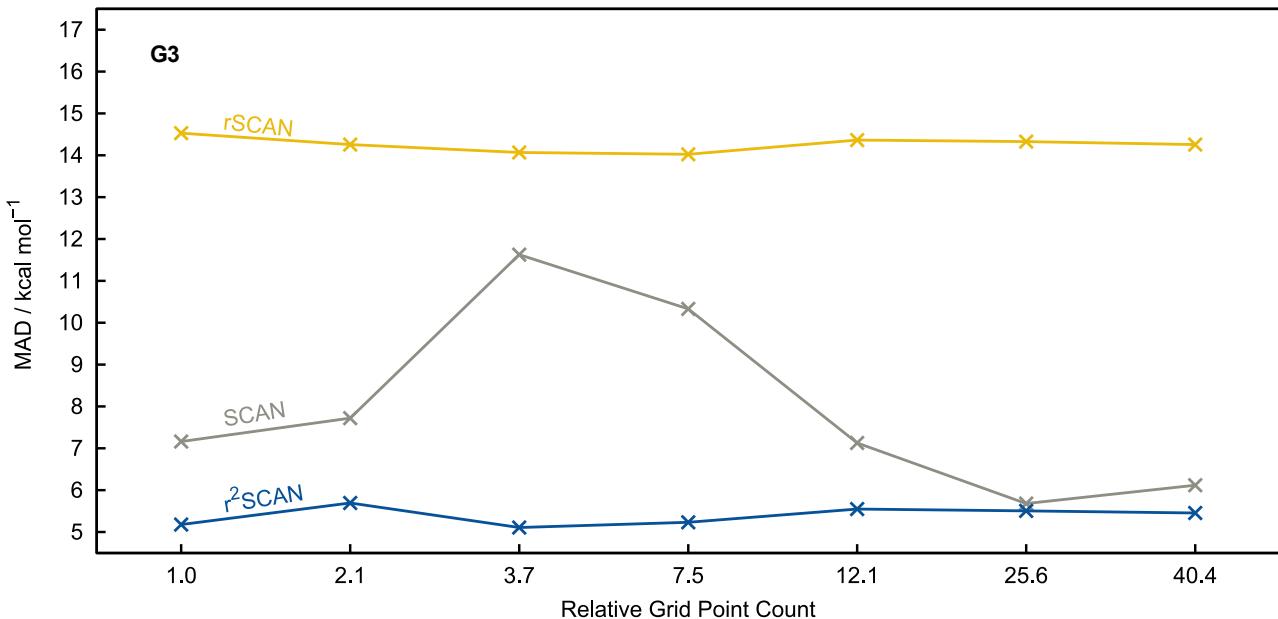
Dispersion
Correction

BSSE
Correction

meta-GGA

Strongly
Constrained and
Appropriately
Normed

2.1 DENSITY FUNCTIONAL r^2 SCAN



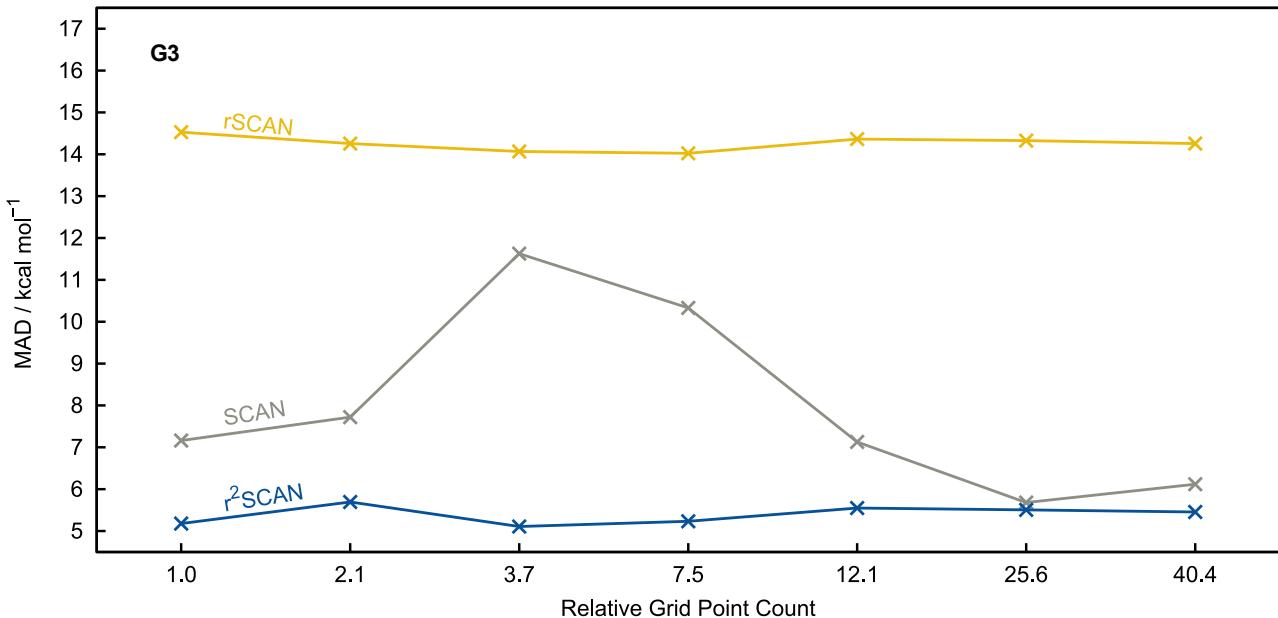
J. Sun, A. Ruzsinszky, J. P. Perdew, *Phys. Rev. Lett.* 2015, 115, 036402.

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J. W. Furness, A. D. Kaplan, J. Ning, J. P. Perdew, J. Sun, *J. Phys. Chem. Lett.* 2020, 11, 19, 8208.

meta-GGA
regularized
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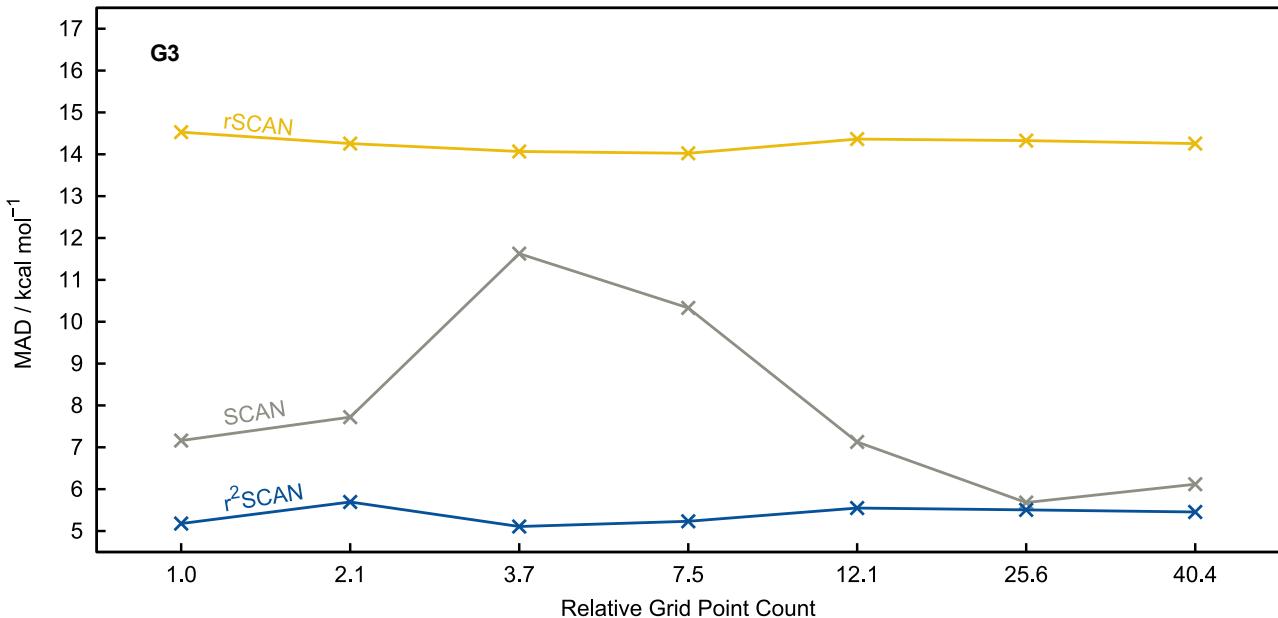
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meta-GGA

regularized-
restored
Strongly
Constrained and
Appropriately
Normed

2.1 DENSITY FUNCTIONAL r^2 SCAN

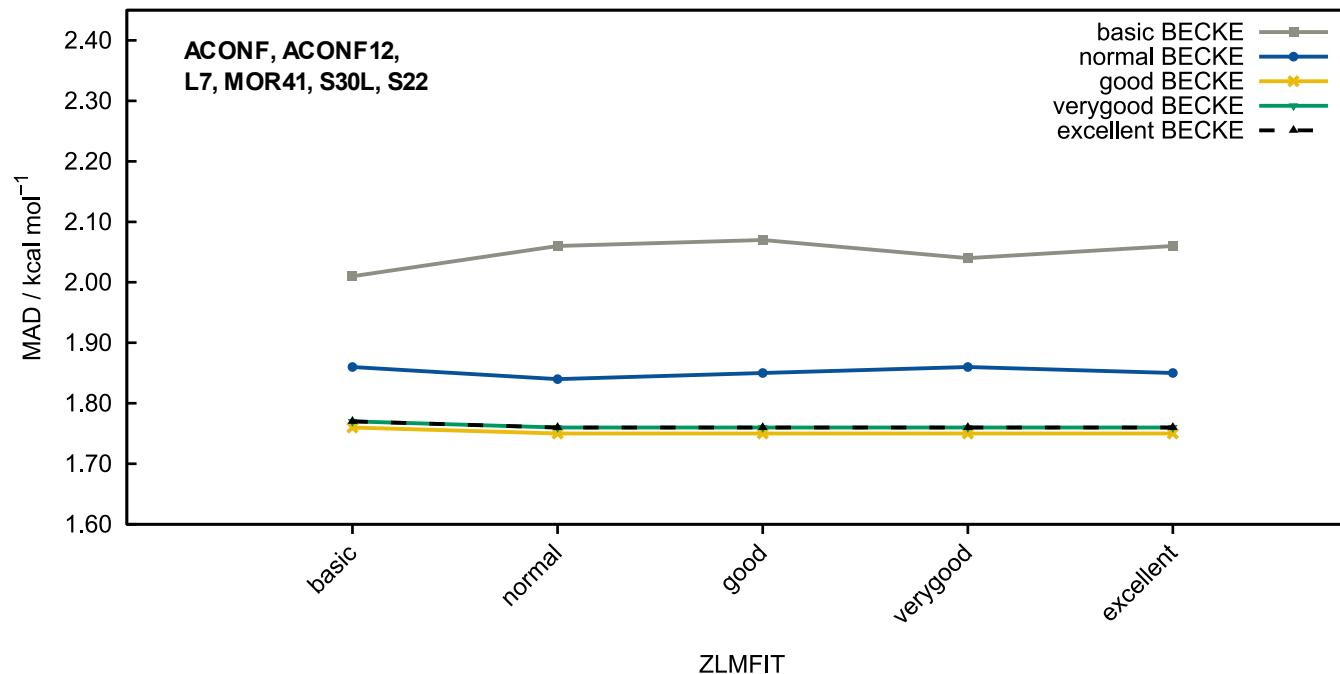


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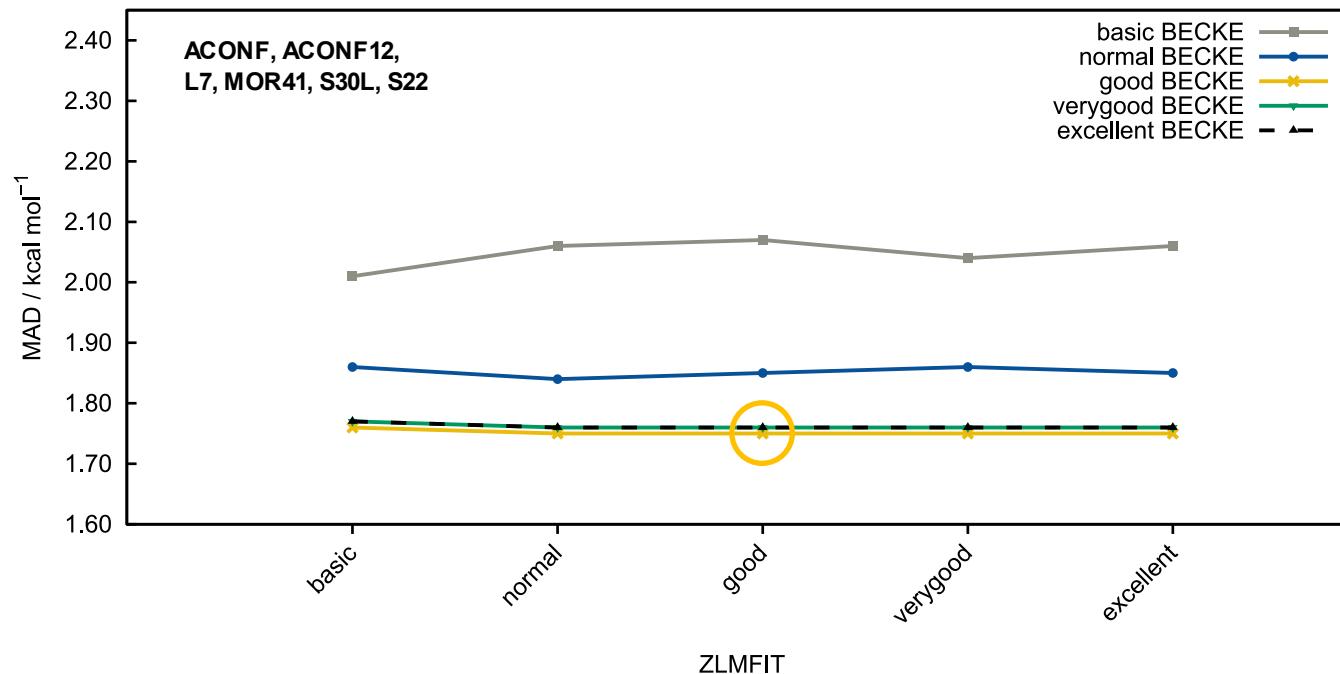
2.1 DENSITY FUNCTIONAL r^2 SCAN



NumericalQuality: Good as default for r^2 SCAN-3c(STO)

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2.1 DENSITY FUNCTIONAL r^2 SCAN



NumericalQuality: Good as default for r^2 SCAN-3c(STO)

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2. r^2 SCAN-3c(STO)

Density
Functional
 r^2 SCAN

Basis Set
mTZ2P

Dispersion
Correction

BSSE
Correction

2.2 BASIS SET mTZ2P

- DZP: H*, He
- TZ2P: N, O*, F, Ne, Si – S, Cl, Ar, Kr
- TZP: remaining elements
- SR-ZORA is used instead of ECPs

Element	Contraction	
	GTO	STO
H	[2s1p]	[2s1p]
C	[5s3p1d]	[5s3p1d]
O	[5s3p2d]	[5s3p1d1f]
I	[6s5p3d]	[12s10p6d]

* H: 2p exponent was changed from 1.25 to 1.70

O: 3d exponent was changed from 2.00 to 2.15

2. r^2 SCAN-3c(STO)

Density
Functional
 r^2 SCAN

Basis Set
mTZ2P

Dispersion
Correction

BSSE
Correction

2.3 GRIMME'S D4 DISPERSION CORRECTION



- Energy & gradient correction
- Three-body interactions included by the ATM term (Axilrod-Teller-Muto)
- Charge information is considered
- Geometry input is required
- Computation in a few seconds

	GTO	STO
s_6	1.00	1.00
s_8	0.00	0.00
s_9	2.00	1.53
a_1	0.42	0.42
a_2	5.65	5.65
β	2.00	2.00
γ	1.00	1.00

2. r^2 SCAN-3c(STO)

Density
Functional
 r^2 SCAN

Basis Set
mTZ2P

Dispersion
Correction

BSSE
Correction

2.4 gCP CORRECTION

- Additive BSSE (& BSIE) correction term
- Energy & gradient correction
- Depends on the basis set
- Geometry input is required
- Computation in a few seconds

σ parameter	
GTO	STO
1.000	0.879

2.4 gCP CORRECTION

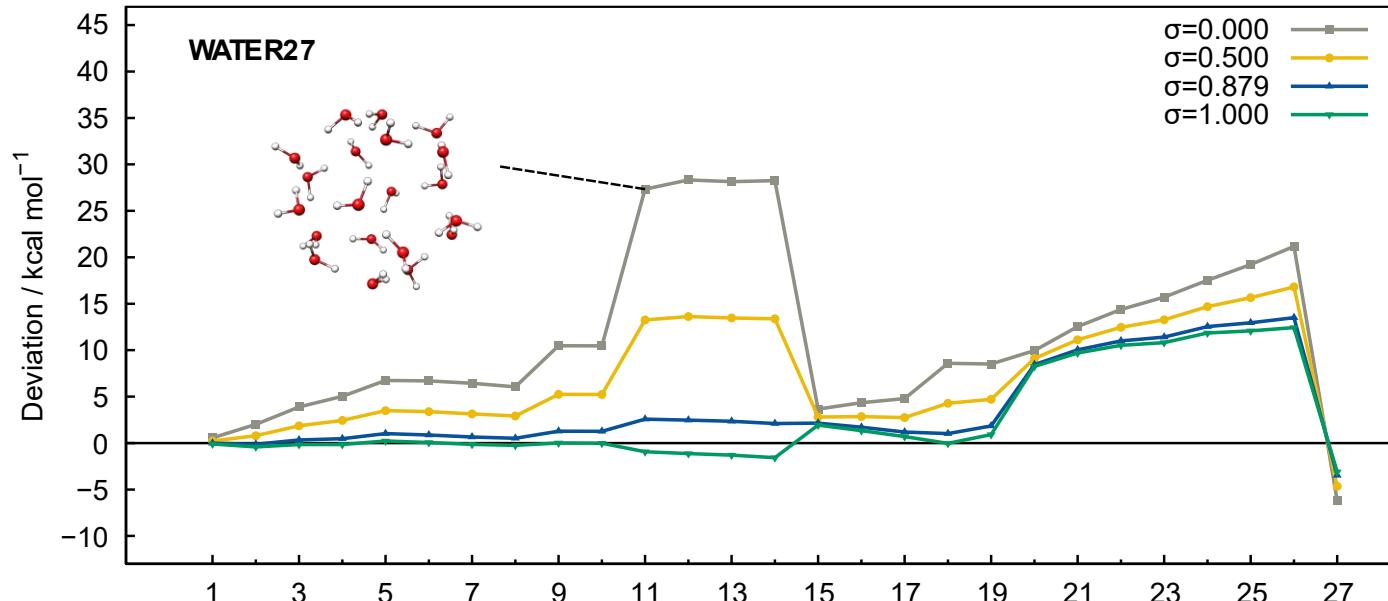


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2. r²SCAN-3c(STO)

Density
Functional
r²SCAN

Basis Set
mTZ2P

Dispersion
Correction

BSSE
Correction

$$E_{\text{tot}}^{\text{r}^2\text{SCAN}-3\text{c}} = E_{\text{tot}}^{\text{r}^2\text{SCAN}} + E_{\text{disp}}^{\text{D4}} + E_{\text{gCP}}$$

3. RESULTS

3.1 GEOMETRY

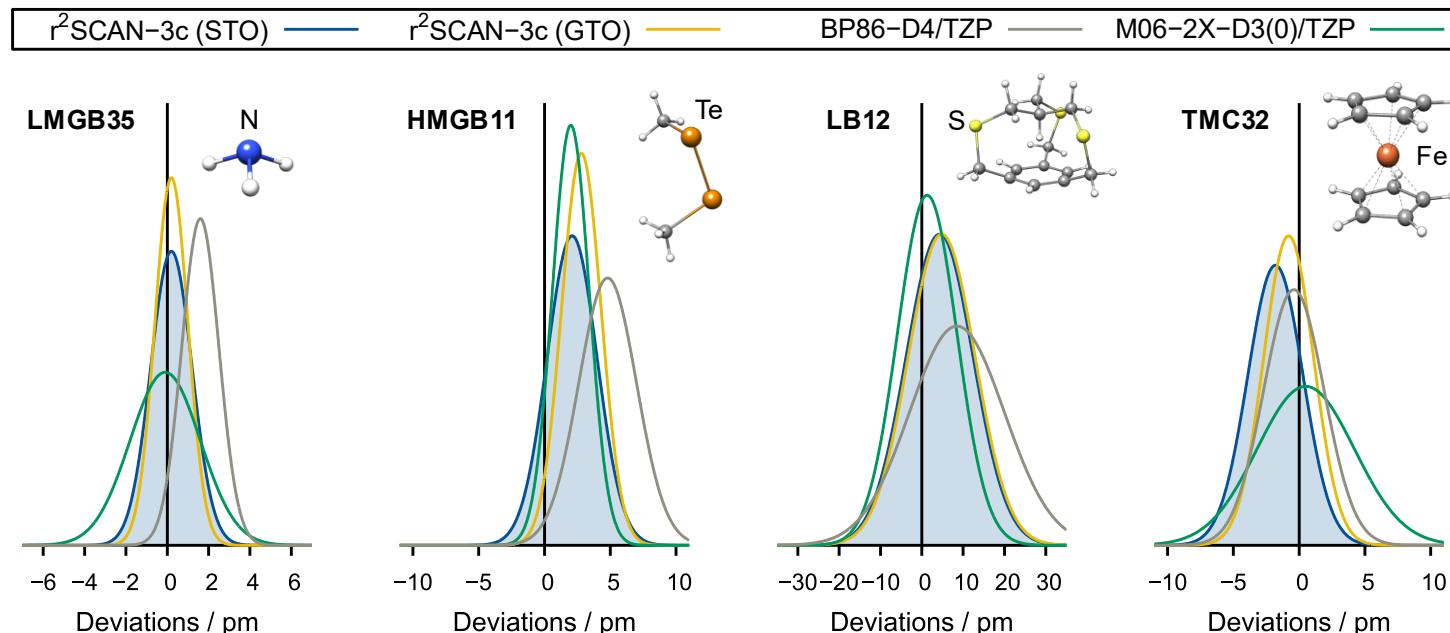
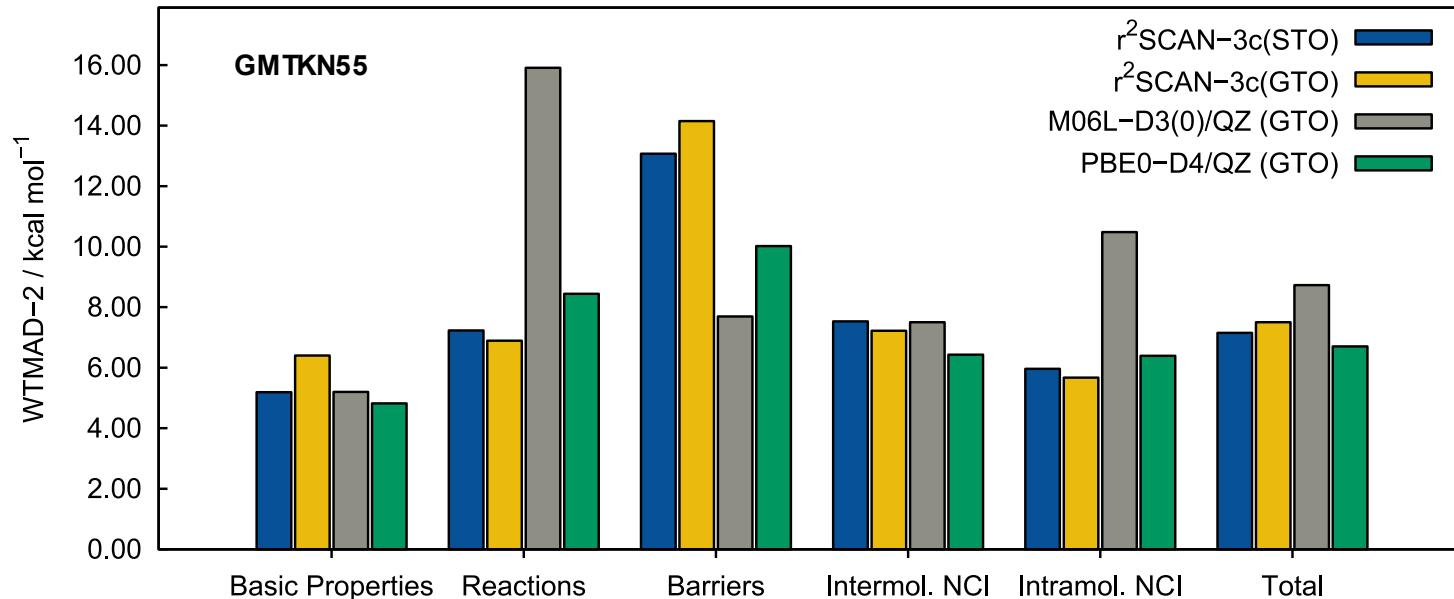


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3.2 GENERAL MAIN-GROUP ENERGIES



$$\text{WTMAD-2} = \frac{1}{\sum_i^n N_i} \sum_i^n N_i \cdot \frac{57.82 \text{ kcal mol}^{-1}}{|\Delta E|_i} \cdot \text{MAD}_i$$

3.3 ION- π INTERACTIONS

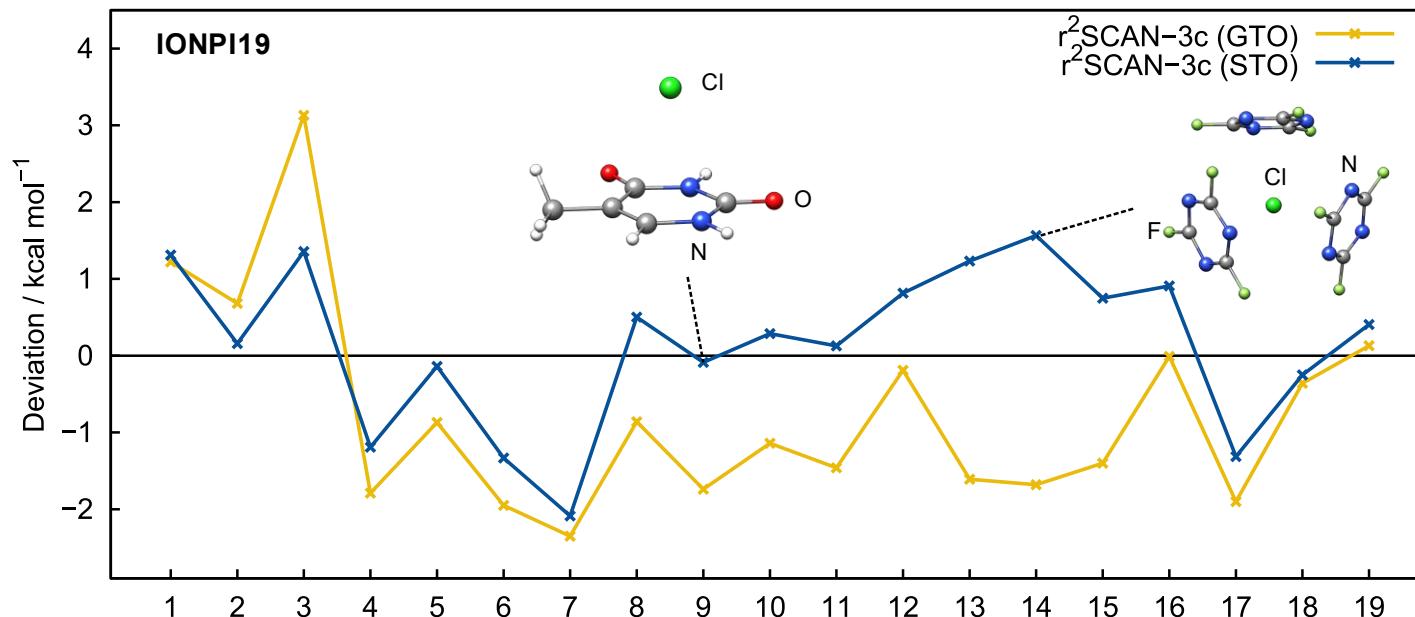


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3.4 CONFORMATIONAL ENERGIES

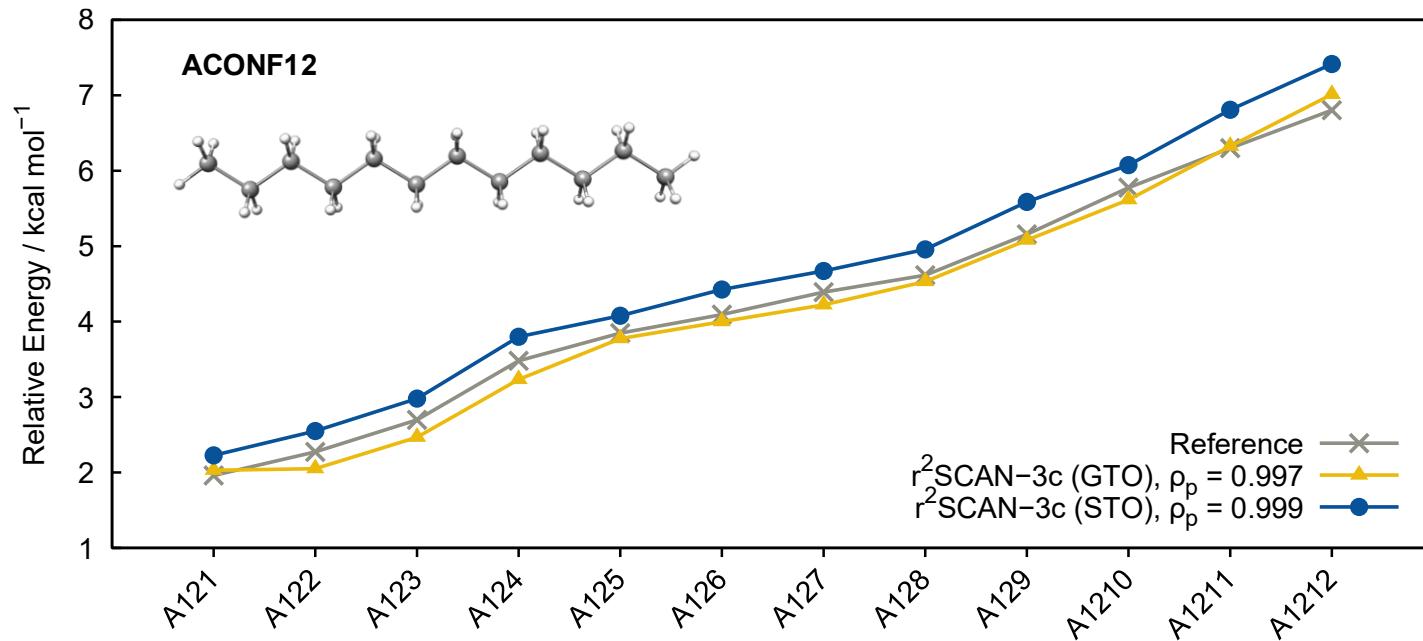


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3.5 ORGANOMETALLIC CHEMISTRY

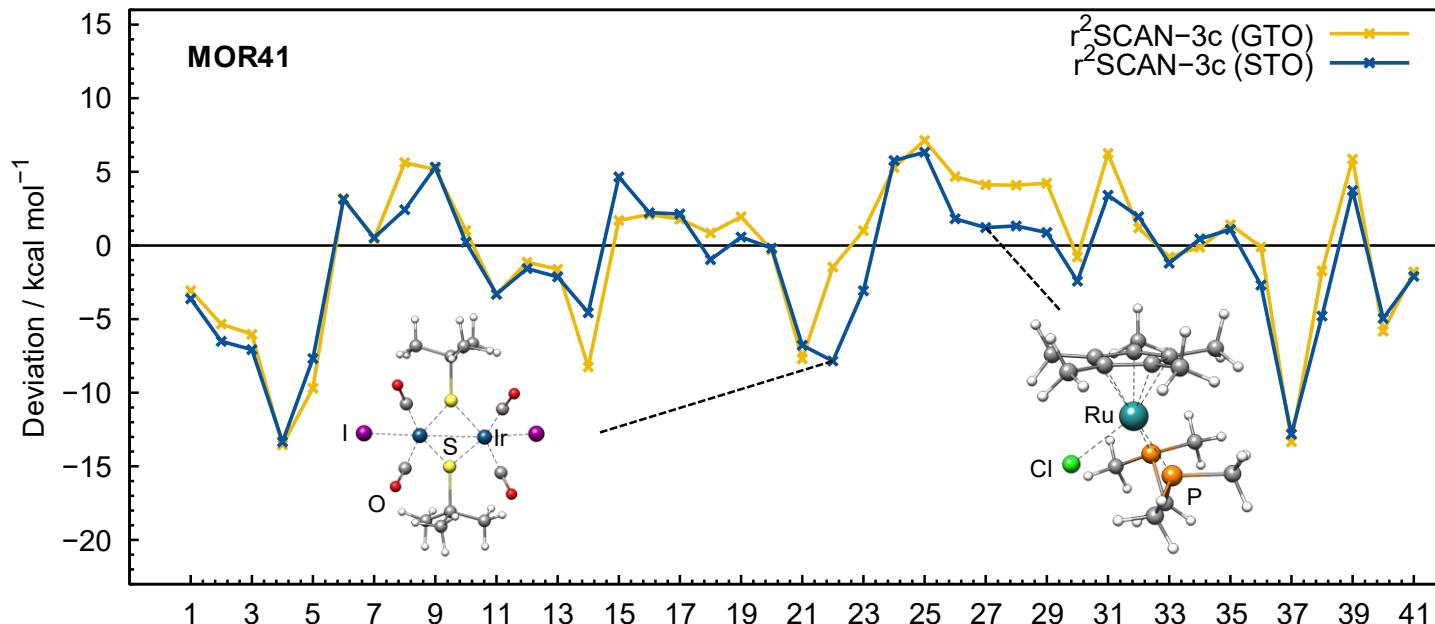


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3.6 COMPUTATION TIME

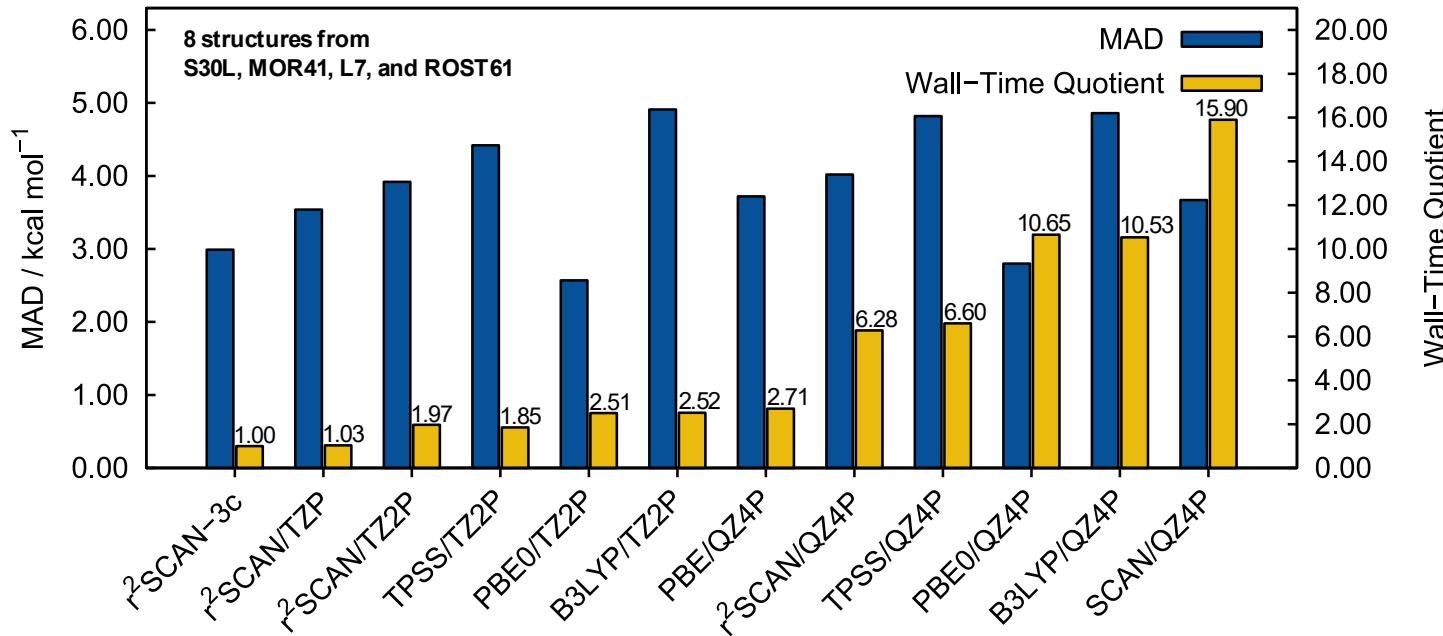


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4. CONCLUSION

4. CONCLUSION

- In comparison to r²SCAN-3c(GTO):
 - Modified mTZ2P basis set, D4 and gCP correction
 - In most cases similar results
- QZ4P quality at the cost of TZP basis set
- Good results for π -interactions & conformational energies
- The versatile “Swiss Army-Knife” r²SCAN-3c(STO) is a valuable tool for everyday problems.
- Available in the next AMS release (2023)



r²SCAN-3c(STO)



r²SCAN-3c(GTO)

5. DEMO

6. ACKNOWLEDGEMENTS

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