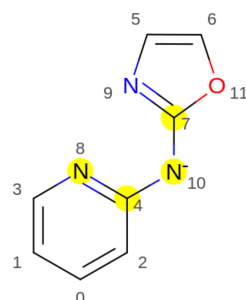


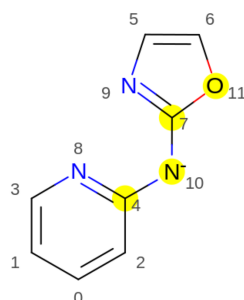
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The methods are listed on the x-axis, and the wall time is shown on the y-axis (log scale).

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~15
default	~15
m05-2x-d3/dzvp	~25
m08-hx-d3/dzvp	~25
m06-2x-d3/dzvp	~30
pw6b95-d3/dzvp	~30
pw6b95-d3bj/dzvp	~30
b3lyp-d3bj/6-31+g**	~35
b3lyp-d3bj/6-311+g**	~38
b3lyp-d3bj/def2-tzvp	~50
b3lyp-d3bj/def2-tzvpp	~52
b3lyp-d3bj/def2-tzvpd	~80
b3lyp-d3bj/def2-tzvppd	~100
mp2/aug-cc-pvtz	~110
heavy-aug-cc-pvtz	~130
b3lyp-d3bj/def2-qzvp	~140
b3lyp-nl/dzvp	~150
wb97m-v/dzvp	~160
df-ccsd(t)/cbs	~15000

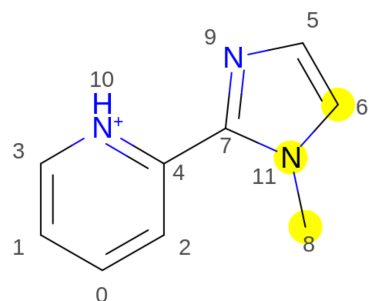
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The methods are listed on the x-axis, and the wall time is shown on the y-axis (log scale).

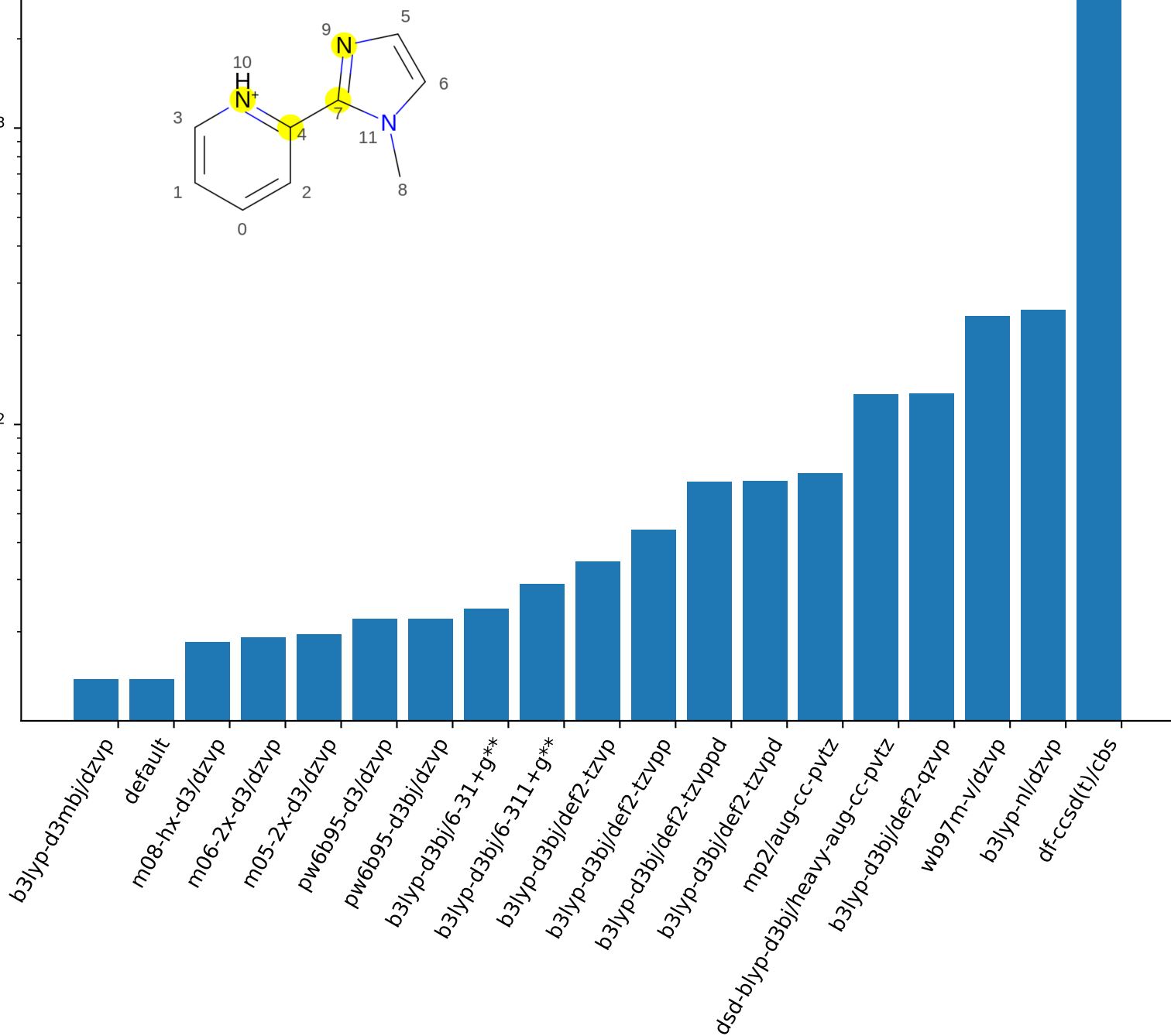
Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~20
default	~20
m08-hx-d3/dzvp	~30
m05-2x-d3/dzvp	~30
m06-2x-d3/dzvp	~30
b3lyp-d3bj/6-31+g**	~35
pw6b95-d3/dzvp	~35
pw6b95-d3bj/dzvp	~35
b3lyp-d3bj/6-311+g**	~45
b3lyp-d3bj/def2-tzvpp	~50
b3lyp-d3bj/def2-tzvp	~60
b3lyp-d3bj/def2-tzvppd	~75
mp2/aug-cc-pvtz	~100
b3lyp-d3bj/def2-qzvp	~130
dsd-blyp-d3bj/heavy-aug-cc-pvtz	~160
b3lyp-nl/dzvp	~170
wb97m-v/dzvp	~180
df-ccsd(t)/cbs	~15000

Wall time in seconds (in log scale)

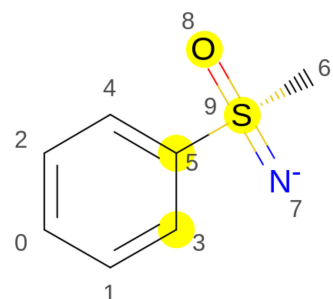


m08-hx-d3/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3mbj/dzvp
default
m06-2x-d3/dzvp
m05-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

Wall time in seconds (in log scale)



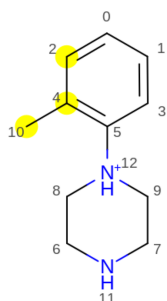
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The methods are listed on the x-axis, and the wall time is shown on the y-axis (log scale).

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~15
default	~15
m06-2x-d3/dzvp	~25
m05-2x-d3/dzvp	~25
m08-hx-d3/dzvp	~25
pw6b95-d3/dzvp	~28
pw6b95-d3bj/dzvp	~28
b3lyp-d3bj/6-31+g**	~35
b3lyp-d3bj/6-311+g**	~40
b3lyp-d3bj/def2-tzvp	~45
b3lyp-d3bj/def2-tzvpp	~65
b3lyp-d3bj/def2-tzvpd	~75
b3lyp-d3bj/def2-tzvppd	~80
mp2/aug-cc-pvtz	~85
d3d-blyp-d3bj/heavy-aug-cc-pvtz	~130
b3lyp-d3bj/def2-qzvp	~140
b3lyp-nl/dzvp	~145
wb97m-v/dzvp	~155
df-ccsd(t)/cbs	~4000

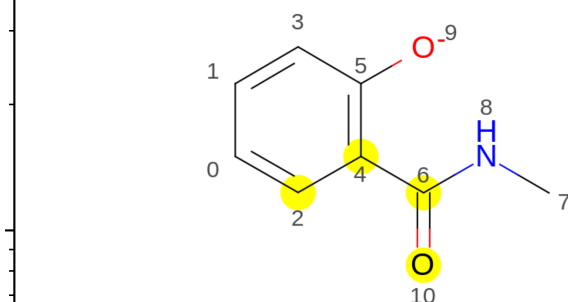
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The y-axis ranges from 10^2 to 10^4 seconds. The x-axis lists the computational methods. The wall time increases significantly for the methods listed from left to right, with the final method, df-ccsd(t)/cbs, showing the highest wall time, exceeding 10^4 seconds.

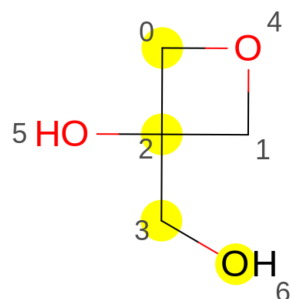
Computational Method	Wall time in seconds (in log scale)
b3lyp-d3mbj/dzvp	~20
default	~20
m05-2x-d3/dzvp	~30
pw6b95-d3/dzvp	~30
pw6b95-d3bj/dzvp	~30
m08-hx-d3/dzvp	~30
m06-2x-d3/dzvp	~30
b3lyp-d3bj/6-31+g**	~30
b3lyp-d3bj/6-311+g**	~40
b3lyp-d3bj/def2-tzvp	~50
b3lyp-d3bj/def2-tzvpp	~70
b3lyp-d3bj/def2-tzvppd	~110
b3lyp-d3bj/def2-tzvppd	~130
mp2/aug-cc-pvtz	~200
b3lyp-d3bj/def2-qzvp	~220
b3lyp-nl/dzvp	~450
wb97m-v/dzvp	~480
df-ccsd(t)/cbs	> 10000

Wall time in seconds (in log scale)



m05-2x-d3/dzvp
m08-hx-d3/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3mbj/dzvp
default
m06-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
d3d-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

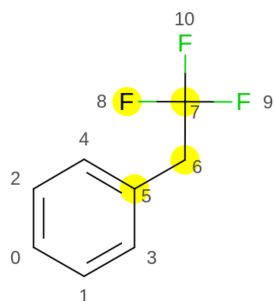
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The Y-axis is logarithmic, ranging from 10¹ to 10² seconds. The X-axis lists the computational methods. The wall time increases significantly for methods involving def2-tzvp and def2-tzvpd basis sets, with df-ccsd(t)/cbs being the most computationally expensive.

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~6.5
default	~6.5
m05-2x-d3/6-31+g**	~8.5
pw6b95-d3/dzvp	~9.0
pw6b95-d3/dzvp	~9.2
m08-hx-d3/dzvp	~9.2
m06-2x-d3/dzvp	~9.3
b3lyp-d3bj/6-311+g**	~11.0
b3lyp-d3bj/def2-tzvp	~15.0
mp2/aug-cc-pvtz	~18.0
b3lyp-d3bj/def2-tzvp	~19.0
b3lyp-d3bj/def2-tzvpd	~21.0
b3lyp-d3bj/def2-tzvpd	~28.0
d3d-blyp-d3bj/heavy-aug-cc-pvtz	~35.0
b3lyp-d3bj/def2-qzvp	~45.0
b3lyp-nl/dzvp	~75.0
wb97m-v/dzvp	~85.0
df-ccsd(t)/cbs	~150.0

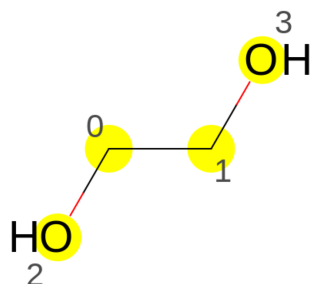
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The Y-axis ranges from 10¹ to 10³ seconds. The X-axis lists the computational methods. The wall time increases significantly for the methods listed on the right side of the chart, reaching over 1000 seconds for the final method.

Computational Method	Wall time in seconds (approx.)
b3lyp-d3mbj/dzvp	9
default	9
m06-2x-d3/dzvp	14
pw6b95-d3/dzvp	14
pw6b95-d3bj/dzvp	14
m08-hx-d3/dzvp	14
m05-2x-d3/dzvp	14
b3lyp-d3bj/6-31+g**	15
b3lyp-d3bj/6-311+g**	17
b3lyp-d3bj/def2-tzvp	23
b3lyp-d3bj/def2-tzvpp	28
b3lyp-d3bj/def2-tzvppd	40
mp2/aug-cc-pvtz	45
b3lyp-d3bj/def2-tzvppd	45
d3d-blyp-d3bj/heavy-aug-cc-pvtz	65
b3lyp-d3bj/def2-qzvp	75
b3lyp-nl/dzvp	125
wb97m-v/dzvp	140
df-ccsd(t)/cbs	1000

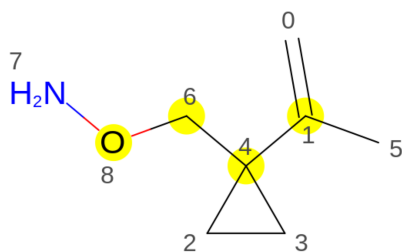
Wall time in seconds (in log scale)



Bar chart showing wall time in seconds (log scale) for various computational methods. The methods are listed on the x-axis, and the wall time is shown on the y-axis (log scale). The methods are ordered by increasing wall time.

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~1.5
default	~1.5
m06-2x-d3/dzvp	~2.5
b3lyp-d3bj/6-31+g**	~3.0
m05-2x-d3/dzvp	~3.5
pw6b95-d3/dzvp	~4.0
pw6b95-d3bj/dzvp	~4.0
m08-hx-d3/dzvp	~4.5
mp2/aug-cc-pvtz	~6.0
b3lyp-d3bj/def2-tzvp	~6.0
b3lyp-d3bj/def2-tzvpp	~7.0
b3lyp-d3bj/def2-tzvpd	~8.0
b3lyp-d3bj/def2-tzvppd	~9.5
dsd-blyp-d3bj/heavy-aug-cc-pvtz	~11.0
b3lyp-d3bj/def2-qzvvp	~18.0
b3lyp-nl/dzvp	~28.0
wb97m-v/dzvp	~38.0
df-ccsd(t)/cbs	~55.0

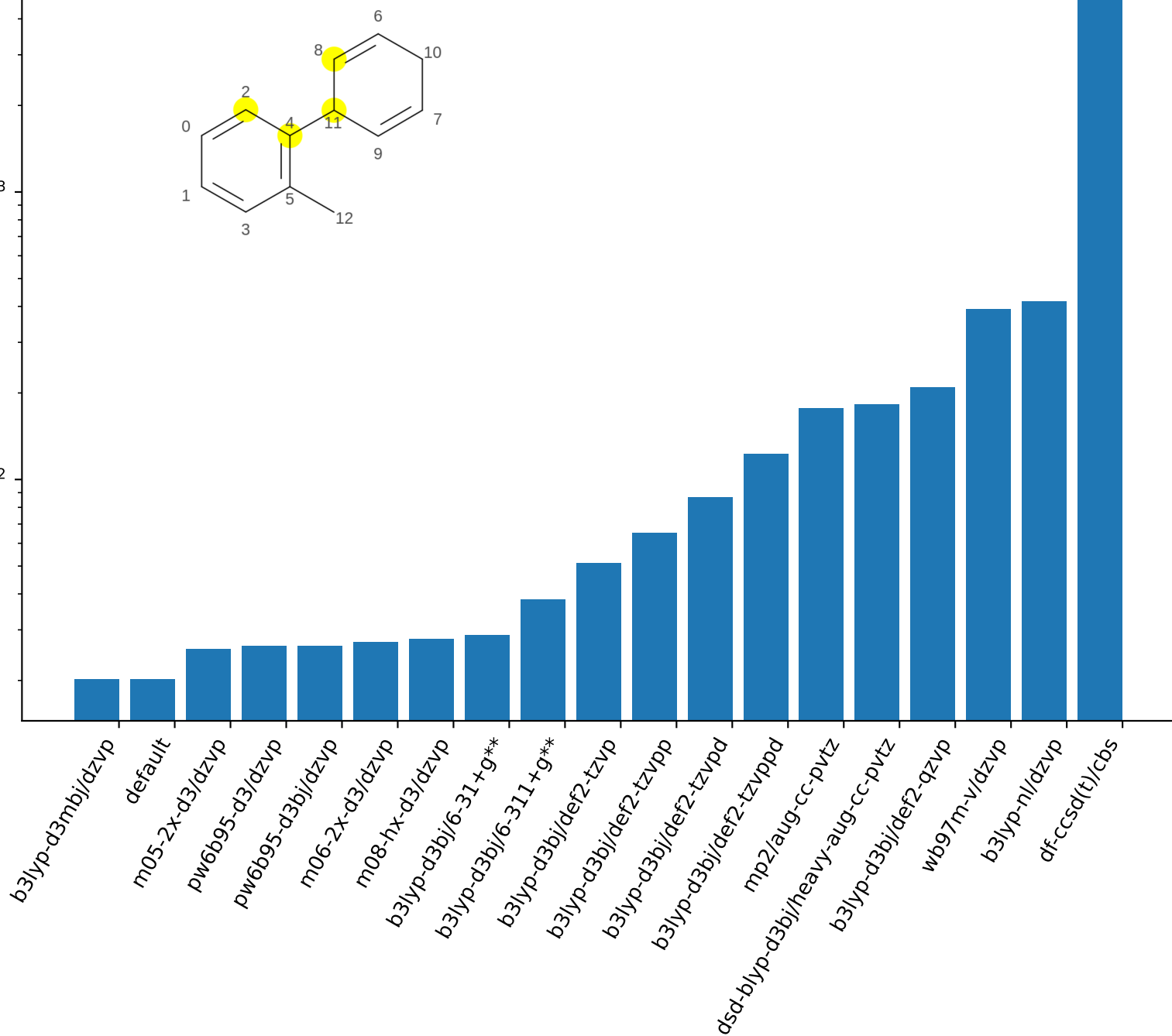
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The Y-axis ranges from 10¹ to 10³ seconds. The X-axis lists the computational methods. The wall time increases significantly for the methods listed on the right side of the chart, reaching over 3000 seconds for df-ccsd(t)/cbs.

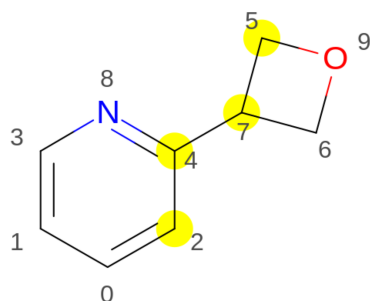
Computational Method	Wall time in seconds (approx.)
b3lyp-d3mbj/dzvp	12
default	12
m05-2x-d3/6-31+g**	15
m05-2x-d3/dzvp	16
m08-hx-d3/dzvp	18
m06-2x-d3/dzvp	19
pw6b95-d3/dzvp	20
pw6b95-d3bj/dzvp	19
b3lyp-d3bj/6-311+g**	21
b3lyp-d3bj/def2-tzvp	28
b3lyp-d3bj/def2-tzvpp	38
mp2/aug-cc-pvtz	48
b3lyp-d3bj/def2-tzvppd	48
b3lyp-d3bj/def2-tzvppd	58
b3lyp-d3bj/heavy-aug-cc-pvtz	75
b3lyp-d3bj/def2-qzvpp	100
b3lyp-nl/dzvp	250
wb97m-v/dzvp	300
df-ccsd(t)/cbs	3500

Wall time in seconds (in log scale)

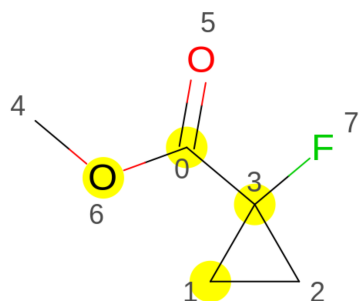


Wall time in seconds (in log scale)

b3lyp-d3mbj/dzvp
default
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-31+g**
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
d3d-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs

10³10²10¹

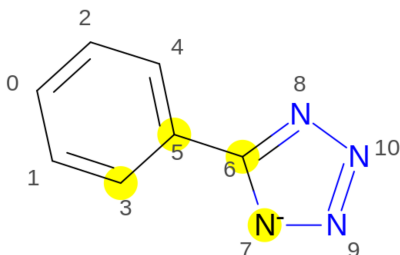
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The methods are listed on the x-axis, and the wall time is shown on the y-axis (log scale).

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	10
default	10
pw6b95-d3/6-31+g**	15
pw6b95-d3/dzvp	18
pw6b95-d3bj/dzvp	18
m05-2x-d3/dzvp	20
m08-hx-d3/dzvp	22
m06-2x-d3/dzvp	22
b3lyp-d3bj/def2-tzvp	23
b3lyp-d3bj/6-311+g**	23
b3lyp-d3bj/def2-tzvpp	28
b3lyp-d3bj/def2-tzvppd	45
b3lyp-d3bj/def2-tzvppd	48
mp2/aug-cc-pvtz	52
d3d-blyp-d3bj/heavy-aug-cc-pvtz	65
b3lyp-d3bj/def2-qzvvp	75
b3lyp-nl/dzvp	110
wb97m-v/dzvp	140
df-ccsd(t)/cbs	3000

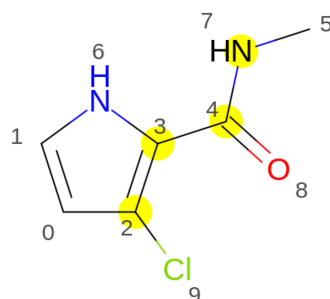
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The methods are listed on the x-axis, and the wall time is shown on the y-axis (log scale).

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~8
default	~8
pw6b95-d3/dzvp	~12
pw6b95-d3bj/dzvp	~12
m05-2x-d3/dzvp	~12
m06-2x-d3/dzvp	~13
m08-hx-d3/dzvp	~13
b3lyp-d3bj/6-31+g**	~16
b3lyp-d3bj/6-311+g**	~17
b3lyp-d3bj/def2-tzvp	~25
b3lyp-d3bj/def2-tzvpp	~30
b3lyp-d3bj/def2-tzvppd	~38
mp2/aug-cc-pvtz	~42
b3lyp-d3bj/def2-tzvppd	~45
d3d-blyp-d3bj/heavy-aug-cc-pvtz	~60
b3lyp-d3bj/def2-qzvp	~68
wb97m-v/dzvp	~88
b3lyp-nl/dzvp	~115
df-ccsd(t)/cbs	~4500

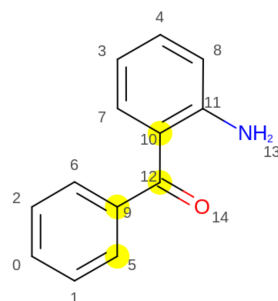
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The Y-axis ranges from 10^1 to 10^3 seconds. The X-axis lists the methods. The wall time increases significantly for the methods listed from left to right, with the final method, df-ccsd(t)/cbs, showing the highest wall time, exceeding 10^3 seconds.

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~9
default	~9
m05-2x-d3/dzvp	~13
pw6b95-d3/dzvp	~13
pw6b95-d3bj/dzvp	~13
m06-2x-d3/dzvp	~14
m08-hx-d3/dzvp	~15
b3lyp-d3bj/6-31+g**	~15
b3lyp-d3bj/6-311+g**	~16
b3lyp-d3bj/def2-tzvp	~22
b3lyp-d3bj/def2-tzvpp	~30
b3lyp-d3bj/def2-tzvppd	~35
mp2/aug-cc-pvtz	~38
b3lyp-d3bj/def2-tzvppd	~42
b3lyp-d3bj/def2-qzvp	~58
dsd-blyp-d3bj/heavy-aug-cc-pvtz	~62
b3lyp-nl/dzvp	~115
wb97m-v/dzvp	~125
df-ccsd(t)/cbs	> 1000

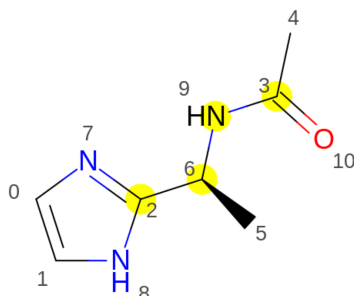
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The methods are listed on the x-axis, and the wall time is shown on the y-axis (log scale).

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~20
default	~20
m05-2x-d3/dzvp	~30
m06-2x-d3/dzvp	~30
m08-hx-d3/dzvp	~30
pw6b95-d3/dzvp	~35
pw6b95-d3bj/dzvp	~35
b3lyp-d3bj/6-31+g**	~38
b3lyp-d3bj/6-311+g**	~45
b3lyp-d3bj/def2-tzvp	~55
b3lyp-d3bj/def2-tzvpp	~65
b3lyp-d3bj/def2-tzvppd	~95
b3lyp-d3bj/def2-tzvppd	~120
mp2/aug-cc-pvtz	~200
dsd-blyp-d3bj/heavy-aug-cc-pvtz	~210
b3lyp-nl/dzvp	~220
wb97m-v/dzvp	~350
df-ccsd(t)/cbs	~3500

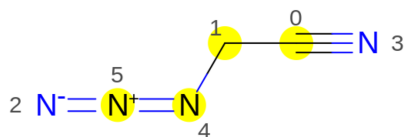
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The methods are listed on the x-axis, and the wall time is shown on the y-axis (log scale).

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~11
default	~11
m08-hx-d3/dzvp	~18
b3lyp-d3bj/6-31+g**	~18
m05-2x-d3/dzvp	~19
pw6b95-d3/dzvp	~20
pw6b95-d3bj/dzvp	~20
m06-2x-d3/dzvp	~21
b3lyp-d3bj/6-311+g**	~22
b3lyp-d3bj/def2-tzvp	~35
b3lyp-d3bj/def2-tzvpp	~42
b3lyp-d3bj/def2-tzvppd	~55
mp2/aug-cc-pvtz	~58
b3lyp-d3bj/def2-tzvppd	~62
b3lyp-d3bj/heavy-aug-cc-pvtz	~95
b3lyp-d3bj/def2-qzvp	~120
b3lyp-nl/dzvp	~250
wb97m-v/dzvp	~260
df-ccsd(t)/cbs	~5000

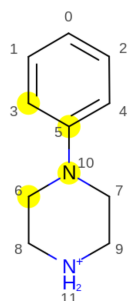
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The methods are listed on the x-axis, and the wall time is shown on the y-axis (log scale, ranging from 10¹ to 10² seconds).

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~2.0
default	~2.0
b3lyp-d3bj/6-31+g**	~2.5
m08-hx-d3/dzvp	~3.5
m05-2x-d3/dzvp	~3.5
m06-2x-d3/dzvp	~3.8
pw6b95-d3/dzvp	~4.0
pw6b95-d3bj/dzvp	~4.0
b3lyp-d3bj/6-311+g**	~4.2
b3lyp-d3bj/def2-tzvp	~5.5
mp2/aug-cc-pvtz	~6.0
b3lyp-d3bj/def2-tzvpp	~6.5
b3lyp-d3bj/def2-tzvppd	~6.5
b3lyp-d3bj/heavy-aug-cc-pvtz	~9.0
b3lyp-d3bj/def2-qzvpp	~15.0
b3lyp-nl/dzvp	~18.0
wb97m-v/dzvp	~25.0
df-ccsd(t)/cbs	~120.0

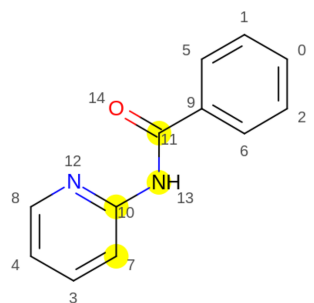
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The y-axis ranges from 10^2 to 10^4 seconds. The x-axis lists the methods. The wall time increases significantly for the methods listed from left to right, with the final method (df-ccsd(t)/cbs) showing the highest wall time, exceeding 10^4 seconds.

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~200
default	~200
m05-2x-d3/dzvp	~220
m08-hx-d3/dzvp	~250
m06-2x-d3/dzvp	~280
pw6b95-d3/dzvp	~300
pw6b95-d3bj/dzvp	~300
b3lyp-d3bj/6-31+g**	~350
b3lyp-d3bj/6-311+g**	~450
b3lyp-d3bj/def2-tzvp	~550
b3lyp-d3bj/def2-tzvpp	~750
b3lyp-d3bj/def2-tzvppd	~850
mp2/aug-cc-pvtz	~1000
b3lyp-d3bj/def2-tzvppd	~1050
d3d-blyp-d3bj/heavy-aug-cc-pvtz	~1800
b3lyp-d3bj/def2-qzvp	~2500
wb97m-v/dzvp	~4500
b3lyp-nl/dzvp	~4800
df-ccsd(t)/cbs	> 10000

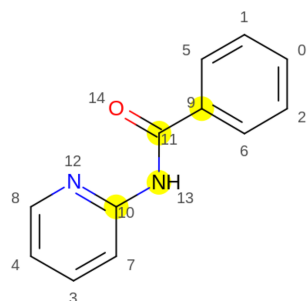
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The y-axis ranges from 10^2 to 10^4 seconds. The x-axis lists the computational methods. The wall time increases significantly for the methods listed from left to right, with the final method (df-ccsd(t)/cbs) showing the highest wall time, exceeding 10^4 seconds.

Computational Method	Wall time in seconds (in log scale)
b3lyp-d3mbj/dzvp	~200
default	~200
m06-2x-d3/dzvp	~300
m08-hx-d3/dzvp	~300
m05-2x-d3/dzvp	~350
pw6b95-d3/dzvp	~380
pw6b95-d3bj/dzvp	~380
b3lyp-d3bj/6-31+g**	~380
b3lyp-d3bj/6-311+g**	~450
b3lyp-d3bj/def2-tzvp	~550
b3lyp-d3bj/def2-tzvpp	~650
b3lyp-d3bj/def2-tzvppd	~850
mp2/aug-cc-pvtz	~1000
b3lyp-d3bj/def2-qzvp	~1500
dsd-blyp-d3bj/heavy-aug-cc-pvtz	~1800
wb97m-v/dzvp	~3500
b3lyp-nl/dzvp	~4000
df-ccsd(t)/cbs	> 10000

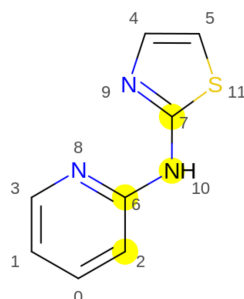
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The methods are listed on the x-axis, and the wall time is plotted on the y-axis (log scale).

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~20
default	~20
m08-hx-d3/dzvp	~22
m05-2x-d3/dzvp	~24
m06-2x-d3/dzvp	~25
pw6b95-d3/dzvp	~26
pw6b95-d3bj/dzvp	~26
b3lyp-d3bj/6-31+g**	~30
b3lyp-d3bj/6-311+g**	~35
b3lyp-d3bj/def2-tzvp	~45
b3lyp-d3bj/def2-tzvpp	~55
b3lyp-d3bj/def2-tzvpd	~75
mp2/aug-cc-pvtz	~90
b3lyp-d3bj/def2-qzvp	~120
heavy-aug-cc-pvtz	~180
wb97m-v/dzvp	~350
b3lyp-nl/dzvp	~350
df-ccsd(t)/cbs	~35000

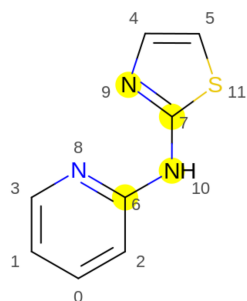
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The methods are listed on the x-axis, and the wall time is shown on the y-axis (log scale).

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~11
default	~11
m08-hx-d3/dzvp	~18
m05-2x-d3/dzvp	~19
pw6b95-d3/dzvp	~19
pw6b95-d3bj/dzvp	~19
m06-2x-d3/dzvp	~20
b3lyp-d3bj/6-31+g**	~22
b3lyp-d3bj/6-311+g**	~25
b3lyp-d3bj/def2-tzvp	~28
b3lyp-d3bj/def2-tzvpp	~38
b3lyp-d3bj/def2-tzvppd	~55
mp2/aug-cc-pvtz	~58
b3lyp-d3bj/def2-tzvppd	~58
d3d-blyp-d3bj/heavy-aug-cc-pvtz	~95
b3lyp-d3bj/def2-qzvp	~100
wb97m-v/dzvp	~180
b3lyp-nl/dzvp	~190
df-ccsd(t)/cbs	~5000

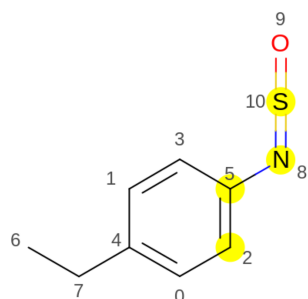
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The y-axis ranges from 10^1 to 10^4 seconds. The x-axis lists the methods. The wall time increases significantly for the methods listed on the right side of the chart.

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~20
default	~20
pw6b95-d3b1/6-31+g**	~30
pw6b95-d3/dzvp	~30
m08-hx-d3b1/dzvp	~30
m06-2x-d3/dzvp	~35
m05-2x-d3/dzvp	~35
b3lyp-d3b1/6-311+g**	~40
b3lyp-d3b1/def2-tzvp	~50
b3lyp-d3b1/def2-tzvpp	~55
b3lyp-d3b1/def2-tzvppd	~75
mp2/aug-cc-pvtz	~95
b3lyp-d3b1/def2-qzvp	~140
dsd-blyp-d3b1/heavy-aug-cc-pvtz	~150
b3lyp-nl/dzvp	~180
wb97m-v/dzvp	~250
df-ccsd(t)/cbs	~15000

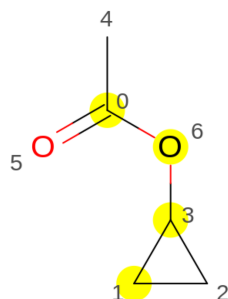
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The methods are listed on the x-axis, and the wall time is shown on the y-axis (log scale).

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~12
default	~12
m05-2x-d3/dzvp	~15
m06-2x-d3/dzvp	~16
m08-hx-d3/dzvp	~17
b3lyp-d3bj/6-31+g**	~18
pw6b95-d3/dzvp	~19
pw6b95-d3bj/dzvp	~19
b3lyp-d3bj/6-311+g**	~25
b3lyp-d3bj/def2-tzvp	~27
b3lyp-d3bj/def2-tzvpp	~35
mp2/aug-cc-pvtz	~55
b3lyp-d3bj/def2-tzvppd	~60
b3lyp-d3bj/heavy-aug-cc-pvtz	~65
b3lyp-d3bj/def2-qzvp	~95
wb97m-v/dzvp	~100
b3lyp-nl/dzvp	~180
df-ccsd(t)/cbs	~450

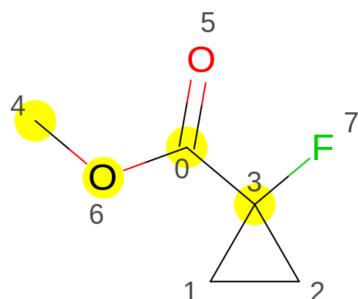
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The methods are listed on the x-axis, and the wall time is shown on the y-axis (log scale).

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~5.5
default	~5.5
m06-2x-d3/dzvp	~8.0
b3lyp-d3bj/6-31+g**	~9.0
m08-hx-d3/dzvp	~9.0
pw6b95-d3/dzvp	~9.0
pw6b95-d3bj/dzvp	~9.0
b3lyp-d3bj/6-311+g**	~9.5
m05-2x-d3/dzvp	~9.5
b3lyp-d3bj/def2-tzvp	~13.0
b3lyp-d3bj/def2-tzvpp	~17.0
b3lyp-d3bj/def2-tzvppd	~20.0
mp2/aug-cc-pvtz	~23.0
b3lyp-d3bj/def2-tzvppd	~24.0
d3d-blyp-d3bj/heavy-aug-cc-pvtz	~30.0
b3lyp-d3bj/def2-qzvpp	~45.0
wb97m-v/dzvp	~75.0
b3lyp-nl/dzvp	~80.0
df-ccsd(t)/cbs	~150.0

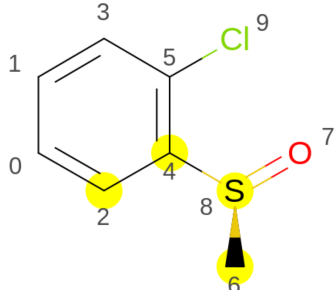
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The y-axis is logarithmic, ranging from 10¹ to 10². The x-axis lists the computational methods. The wall time increases significantly for the methods listed on the right side of the chart.

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~7.5
default	~7.5
m05-2x-d3/dzvp	~9.0
m06-2x-d3/dzvp	~9.5
m08-hx-d3/dzvp	~9.8
b3lyp-d3bj/6-31+g**	~10.0
pw6b95-d3/dzvp	~10.0
pw6b95-d3bj/dzvp	~10.0
b3lyp-d3bj/6-311+g**	~11.5
b3lyp-d3bj/def2-tzvp	~16.0
b3lyp-d3bj/def2-tzvpp	~17.0
mp2/aug-cc-pvtz	~21.0
b3lyp-d3bj/def2-tzvpd	~22.0
b3lyp-d3bj/def2-tzvppd	~25.0
d3d-blyp-d3bj/heavy-aug-cc-pvtz	~38.0
b3lyp-d3bj/def2-qzvvp	~55.0
wb97m-v/dzvp	~85.0
b3lyp-nl/dzvp	~85.0
df-ccsd(t)/cbs	~100.0

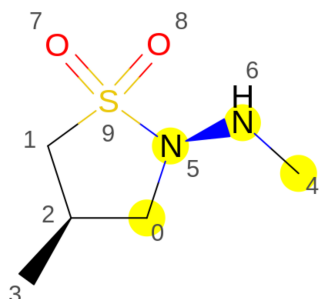
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The x-axis lists the methods, and the y-axis shows the wall time in seconds on a logarithmic scale from 10¹ to 10³.

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~8.5
default	~8.5
m06-2x-d3/dzvp	~13.5
b3lyp-d3bj/6-31+g**	~14.5
pw6b95-d3/dzvp	~14.5
pw6b95-d3bj/dzvp	~14.5
m08-hx-d3/dzvp	~14.5
m05-2x-d3/dzvp	~15.5
b3lyp-d3bj/6-311+g**	~20.5
b3lyp-d3bj/def2-tzvp	~23.5
b3lyp-d3bj/def2-tzvpp	~28.5
b3lyp-d3bj/def2-tzvppd	~40.5
mp2/aug-cc-pvtz	~45.5
b3lyp-d3bj/def2-tzvppd	~50.5
b3lyp-d3bj/heavy-aug-cc-pvtz	~65.5
b3lyp-d3bj/def2-qzvp	~75.5
wb97m-v/dzvp	~115.5
b3lyp-nl/dzvp	~125.5
df-ccsd(t)/cbs	~3500.5

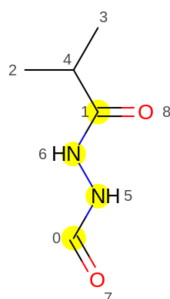
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The Y-axis ranges from 10^1 to 10^4 seconds. The X-axis lists the computational methods. The wall time increases significantly for the methods listed on the right side of the chart, reaching over 10^4 seconds for the final method.

Computational Method	Wall time in seconds (approx.)
b3lyp-d3mbj/dzvp	20
default	20
m05-2x-d3/dzvp	30
m08-hx-d3/dzvp	35
pw6b95-d3/dzvp	40
pw6b95-d3bj/dzvp	40
m06-2x-d3/dzvp	40
b3lyp-d3bj/6-311+g**	45
b3lyp-d3bj/def2-tzvp	60
b3lyp-d3bj/def2-tzvpp	70
b3lyp-d3bj/def2-tzvppd	90
mp2/aug-cc-pvtz	120
heavy-aug-cc-pvtz	130
b3lyp-d3bj/def2-qzvp	180
b3lyp-nl/dzvp	350
wb97m-v/dzvp	400
df-ccsd(t)/cbs	10000

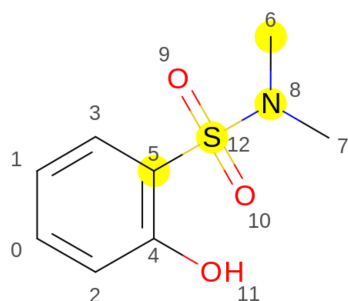
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The Y-axis ranges from 10¹ to 10³ seconds. The X-axis lists the computational methods. The wall time increases significantly for the methods listed on the right side of the chart.

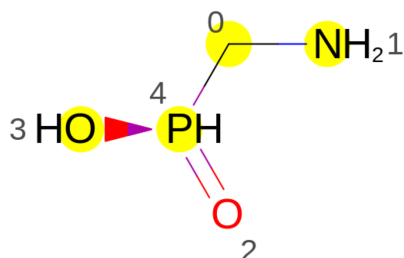
Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~10
default	~10
m05-2x-d3/dzvp	~15
b3lyp-d3bj/6-31+g**	~15
m06-2x-d3/dzvp	~16
m08-hx-d3/dzvp	~16
pw6b95-d3/dzvp	~16
pw6b95-d3bj/dzvp	~16
b3lyp-d3bj/6-311+g**	~18
b3lyp-d3bj/def2-tzvp	~25
b3lyp-d3bj/def2-tzvpp	~30
b3lyp-d3bj/def2-tzvppd	~40
mp2/aug-cc-pvtz	~45
d3d-blyp-d3bj/heavy-aug-cc-pvtz	~55
b3lyp-d3bj/def2-qzvvp	~75
b3lyp-nl/dzvp	~160
wb97m-v/dzvp	~190
df-ccsd(t)/cbs	~3500

Wall time in seconds (in log scale)



b3lyp-d3mbj/dzvp
default
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m08-hx-d3/dzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
dsd-blyp-d3bj/heavy-aug-cc-pvtz
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs

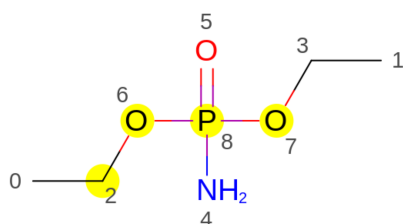
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The Y-axis is logarithmic, ranging from 10¹ to 10². The X-axis lists the computational methods. The wall time increases significantly for the methods listed on the right side of the chart.

Computational Method	Wall time in seconds (in log scale)
b3lyp-d3mbj/dzvp	~5.5
default	~5.5
m08-hx-d3/dzvp	~9.0
m06-2x-d3/dzvp	~9.0
m05-2x-d3/dzvp	~9.5
b3lyp-d3bj/6-311+g**	~10.0
b3lyp-d3bj/6-31+g**	~10.0
pw6b95-d3/dzvp	~10.5
pw6b95-d3bj/dzvp	~10.5
b3lyp-d3bj/def2-tzvp	~15.5
b3lyp-d3bj/def2-tzvpp	~16.5
b3lyp-d3bj/def2-tzvppd	~17.5
mp2/aug-cc-pvtz	~18.5
b3lyp-d3bj/def2-tzvppd	~21.5
b3lyp-d3bj/heavy-aug-cc-pvtz	~28.5
b3lyp-d3bj/def2-qzvpp	~38.5
wb97m-v/dzvp	~55.5
b3lyp-nl/dzvp	~58.5
df-ccsd(t)/cbs	~100.0

Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The methods are listed on the x-axis, and the wall time is shown on the y-axis (log scale).

Method	Wall time (seconds)
b3lyp-d3mbj/dzvp	~15
default	~15
m05-2x-d3/6-31+g**	~25
m06-2x-d3/dzvp	~25
m08-hx-d3/dzvp	~26
pw6b95-d3/dzvp	~28
pw6b95-d3bj/dzvp	~28
b3lyp-d3bj/6-311+g**	~35
b3lyp-d3bj/def2-tzvp	~38
b3lyp-d3bj/def2-tzvpp	~45
b3lyp-d3bj/def2-tzvppd	~70
b3lyp-d3bj/def2-tzvppd	~85
mp2/aug-cc-pvtz	~120
heavy-aug-cc-pvtz	~125
b3lyp-d3bj/def2-qzvp	~135
wb97m-v/dzvp	~220
b3lyp-nl/dzvp	~400
df-ccsd(t)/cbs	~6000

mol: 58, CPU: AMD EPYC 7601 32-Core Processor, # of threads: 4

