# Azobenzene as an effective ligand in Europium chemistry – a synthetic and theoretical study.

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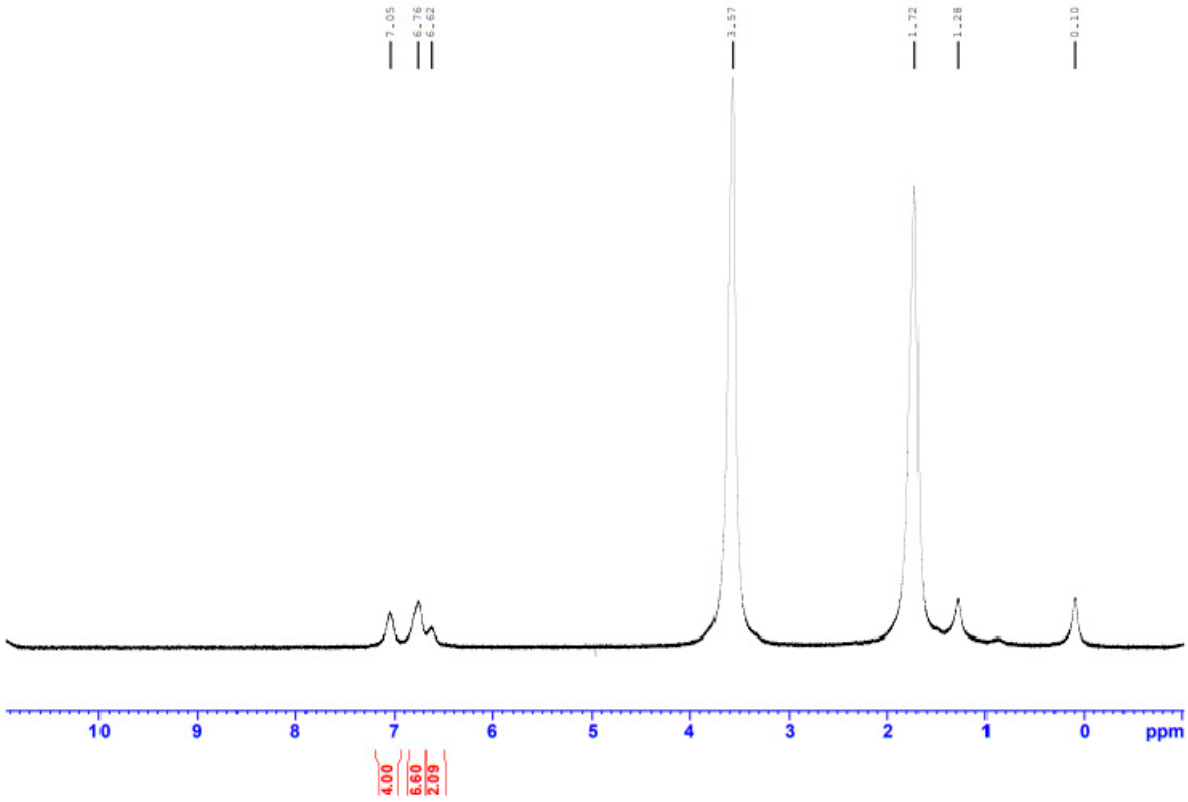



Figure S1. $^{1}$H-NMR spectrum for $[Eu(thf)_3]_2(Ph_2N_2)_2$. Peaks from the phenyl substituents are integrated in the downfield region. Large peaks observed at 3.57 and 1.72 ppm are indicative of excess THF solvent and smaller peaks found at 1.28 and 0.10 ppm arose from vacuum grease contamination.

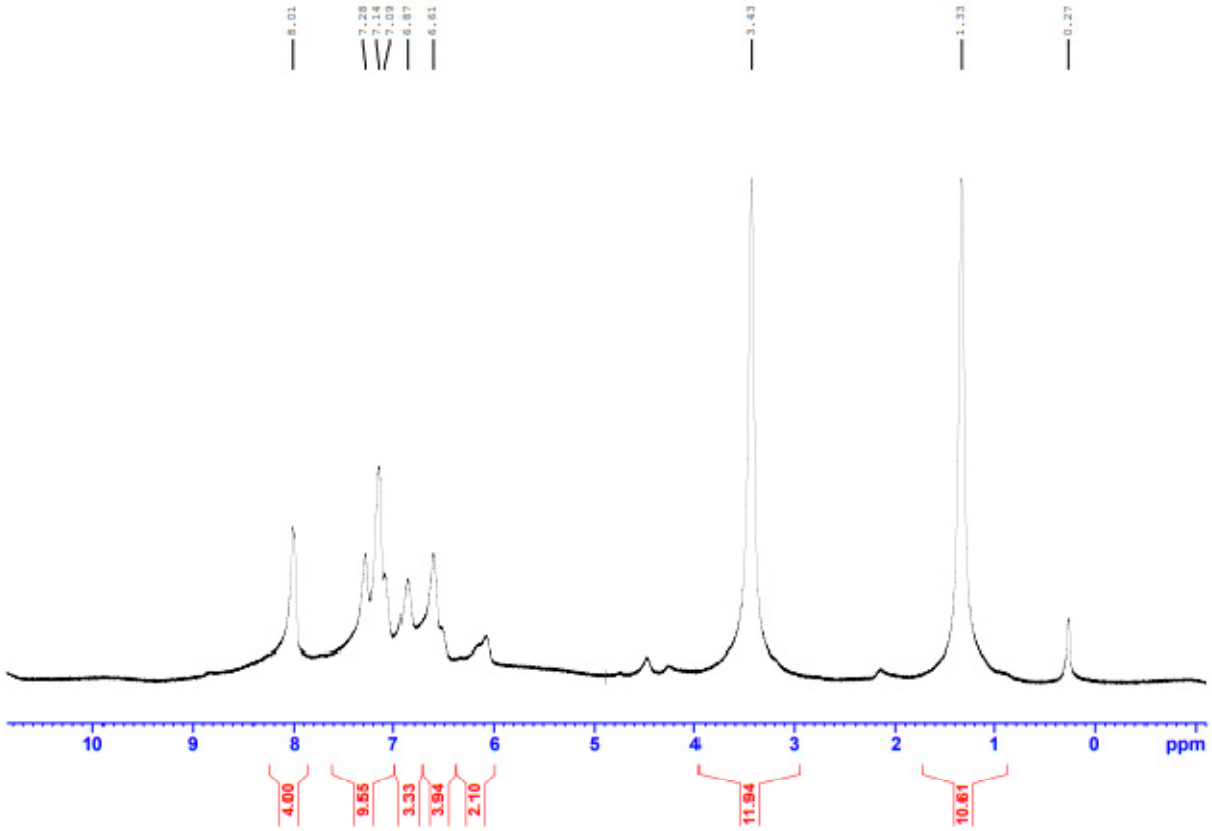



Figure S2. $^{1}$H-NMR spectrum for $[Eu(dme)_2]_2(Ph_2N_2)_2$. Peaks from the phenyl substituents are integrated in the downfield region. Additional splitting is observed due to agostic interactions. Large peaks observed at 3.57 and 1.72 ppm are indicative of excess THF solvent and a smaller peak at 0.27 ppm arose from vacuum grease contamination.

**Table S1**. Crystallographic data and details of measurements for compounds **1** and **2**. Mo Kα (λ=0.71073Å). R1= Σ/ $|F_o|$- $|F_c|$/|Σ|$F_d$; wR2 = $[\Sigma_w(F_o^2-F_2^2)^2/\Sigma_w(F_o^2)^2]^{1/2}$

| **Compound** | **$[Eu(thf)_3]_2(N_2Ph_2)_2$ AV11** | **$[Eu(dme)_2]_2(N_2Ph_2)_2$** |
|---|---|---|
| Formula | $C_{48}H_{68}N_4O_6Eu_2$ | $C_{40}H_{60}N_4O_8Eu_2$ |
| Fw (g $mol^{-1}$) | 1100.98 | 1028.84 |
| *a* (Å) | 10.9632(7) | 10.4832(16) |
| *b* (Å) | 13.5363(9) | 10.8003(19) |
| *c* (Å) | 15.7256(10) | 19.632(3) |
| *α* (°) | 90 | 74.286(4) |
| *β* (°) | 91.565(1) | 89.440(4) |
| *γ* (°) | 90 | 77.989(4) |
| *V* ($Å^3$) | 2332.8(3) | 2090.3(6) |
| *Z* | 2 | 2 |
| Crystal size (mm) | 0.36 × 0.3 × 0.26 | 0.32 × 0.25 × 0.22 |
| Crystal habit | Block, orange | Block, orange |
| Crystal system | Monoclinic | Triclinic |
| Space group | $P2_1/n$ | *P*-1 |
| $d_{calc}$ ( Mg $m^{-3}$) | 1.567 | 1.635 |
| *μ* ($mm^{-1}$) | 2.72 | 3.03 |
| Radiation type | Mo $K_\alpha$ | Mo $K_\alpha$ |
| Wavelength (Å) | 0.71073 | 0.71073 |
| *T* (K) | 100(2) | 100(2) |
| *θ* range (°) | 2.2–30.2 | 2.5–21.4 |
| *F*(000) | 1116 | 1036 |
| $T_{min}$, $T_{max}$ | 0.601, 0.746 | 0.603, 0.746 |
| $R_{int}$ | 0.021 | 0.132 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 16070, 4110, 3803 | 31350, 12867, 6794 |
| independent reflections | 4110 | 12867 |
| No. of parameters, restraints | 271, 0 | 495, 0 |
| Δρmax, Δρmin (e $Å^{-3}$) | 1.57, -0.33 | 1.33, -1.35 |
| R1, wR2 (all data) | R1 = 0.0266<br>wR2 = 0.0606 | R1 = 0.1572<br>wR2 = 0.0865 |
| R1, wR2 (>2*σ*) | R1 = 0.0240<br>wR2 = 0.0587 | R1 = 0.0629<br>wR2 = 0.1088 |

Table S2. The following 32 pages contain the .xyz coordinates for the 16 optimized geometries of structure **1** (containing 128 atoms). Each .xyz file comment line contains the structure name and symmetry (Eu_thf_3_2_N2Ph2_2_AV11__Ci__), then (a) density functional, (b) dispersion correction, (c) C/H/O/N basis set, and (d) effective core potential for the Eu atom. For the first structure, the naming convention is as:
Eu_thf_3_2_N2Ph2_2_AV11__Ci__(a)b3lyp_(b)GD3BJ_(c)Def2SVP_(d)MWB53

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128
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128
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| 1 | -2.67581416 | 2.75267057 | 1.79407762 |
| 1 | -3.67309265 | 1.56505596 | 2.66651001 |

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128
Eu_thf_3_2_N2Ph2_2_AV11__Ci__b3lyp__Def2SVP_MWB53
63       0.38034858       0.09644543      -1.76043087
8       -1.35975438       0.26191350      -3.80524774
8        1.99153873       1.61236915      -3.32157870
8        1.79594030      -1.56051647      -3.42853190
7       -0.68314674      -1.65659392       0.10353346
7        0.75608593      -1.60520837       0.07402787
6       -1.32245396      -2.52637884      -0.73026844
6       -0.68202805      -3.51122433      -1.54596217
1        0.40019600      -3.62279433      -1.47714134
6       -1.42383887      -4.35742562      -2.37544247
1       -0.89413019      -5.11185042      -2.96768235
6       -2.81919264      -4.28011248      -2.44919158
1       -3.38798933      -4.95518979      -3.09254378
6       -3.46902000      -3.31933368      -1.65400842
1       -4.56036625      -3.23602284      -1.68705717
6       -2.75177028      -2.46376822      -0.82634144
1       -3.27393345      -1.71428079      -0.22427589
6        1.45575164      -2.53016296       0.79570742
6        2.87298854      -2.36858627       0.92691572
1        3.33762661      -1.50439971       0.44246663
6        3.64859989      -3.26416524       1.65462769
1        4.72923531      -3.09937122       1.72229206
6        3.07007221      -4.37000208       2.30265681
1        3.68432402      -5.07587415       2.86643270
6        1.68655992      -4.54831845       2.18753321
1        1.21176840      -5.41124714       2.66701190
6        0.88899005      -3.66110285       1.45961904
1       -0.18052705      -3.84582159       1.36301116
6       -2.29591907      -0.76453732      -4.18116941
1       -2.25480102      -1.56578455      -3.43101580
1       -2.01436891      -1.18149968      -5.16784366
6       -3.63306432      -0.03823359      -4.24641108
1       -4.02750067       0.09665696      -3.22702302
1       -4.38478966      -0.58204286      -4.83761386
6       -3.23471547       1.31312515      -4.86287166
1       -3.89222160       2.13607831      -4.54991738
1       -3.26318682       1.25666950      -5.96299057
6       -1.79142794       1.52642487      -4.36573536
1       -1.10872518       1.80803948      -5.18627691
1       -1.72342229       2.28670741      -3.57507360
6        2.18547741       1.50358389      -4.73327978
1        1.38032701       0.87528754      -5.13821082
1        3.15027557       1.00064100      -4.93312055
6        2.18879619       2.95228786      -5.27271415
1        1.25538299       3.18422936      -5.80622127
1        3.01645796       3.10423871      -5.98178372
6        2.33726601       3.82593332      -4.00031786
1        3.11597100       4.59659735      -4.09725811
1        1.38912825       4.33124743      -3.76448822
6        2.66553577       2.80805837      -2.90524782
1        3.75415715       2.61149316      -2.84927392
1        2.29741847       3.06515241      -1.90469104
6        1.30563849      -2.40321993      -4.48751645
1        1.34753337      -1.84097378      -5.43897065
1        0.25845773      -2.66464749      -4.27528480
6        2.23235520      -3.61934242      -4.51043614
1        2.29991402      -4.07999995      -5.50721335
1        1.87090814      -4.38487649      -3.80521174
6        3.55826327      -3.02513029      -4.01779046
1        4.24623731      -3.77539615      -3.60124305
1        4.07825739      -2.50625938      -4.84049289
6        3.08156365      -2.02557430      -2.96459129
1        2.95663602      -2.49764204      -1.97576910
1        3.74651757      -1.15389336      -2.85460105
63      -0.35914546       0.15988270       1.82271212
8        1.38095750      -0.00558537       3.86752899
8       -1.97033560      -1.35604103       3.38385995
8       -1.77473718       1.81684460       3.49081315
7        0.70434986       1.91292204      -0.04125221
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| 6 | 0.70323117 | 3.76755246 | 1.60824342 |
| 1 | -0.37899287 | 3.87912246 | 1.53942259 |
| 6 | 1.44504200 | 4.61375374 | 2.43772372 |
| 1 | 0.91533332 | 5.36817855 | 3.02996360 |
| 6 | 2.84039576 | 4.53644061 | 2.51147283 |
| 1 | 3.40919246 | 5.21151791 | 3.15482503 |
| 6 | 3.49022312 | 3.57566180 | 1.71628967 |
| 1 | 4.58156937 | 3.49235096 | 1.74933842 |
| 6 | 2.77297341 | 2.72009635 | 0.88862269 |
| 1 | 3.29513657 | 1.97060891 | 0.28655714 |
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| 6 | -2.85178541 | 2.62491439 | -0.86463447 |
| 1 | -3.31642349 | 1.76072784 | -0.38018538 |
| 6 | -3.62739677 | 3.52049336 | -1.59234644 |
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| 6 | -3.04886909 | 4.62633020 | -2.24037556 |
| 1 | -3.66312090 | 5.33220228 | -2.80415145 |
| 6 | -1.66535679 | 4.80464657 | -2.12525196 |
| 1 | -1.19056528 | 5.66757526 | -2.60473065 |
| 6 | -0.86778692 | 3.91743097 | -1.39733779 |
| 1 | 0.20173018 | 4.10214972 | -1.30072991 |
| 6 | 2.31712220 | 1.02086545 | 4.24345066 |
| 1 | 2.27600414 | 1.82211267 | 3.49329705 |
| 1 | 2.03557203 | 1.43782780 | 5.23012491 |
| 6 | 3.65426744 | 0.29456171 | 4.30869233 |
| 1 | 4.04870380 | 0.15967116 | 3.28930427 |
| 1 | 4.40599279 | 0.83837098 | 4.89989511 |
| 6 | 3.25591860 | -1.05679703 | 4.92515291 |
| 1 | 3.91342473 | -1.87975018 | 4.61219863 |
| 1 | 3.28438994 | -1.00034138 | 6.02527182 |
| 6 | 1.81263107 | -1.27009674 | 4.42801661 |
| 1 | 1.12992830 | -1.55171136 | 5.24855816 |
| 1 | 1.74462541 | -2.03037929 | 3.63735485 |
| 6 | -2.16427428 | -1.24725576 | 4.79556103 |
| 1 | -1.35912389 | -0.61895941 | 5.20049207 |
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| 6 | -2.16759306 | -2.69595974 | 5.33499540 |
| 1 | -1.23417986 | -2.92790123 | 5.86850252 |
| 1 | -2.99525484 | -2.84791059 | 6.04406497 |
| 6 | -2.31606289 | -3.56960519 | 4.06259911 |
| 1 | -3.09476787 | -4.34026922 | 4.15953936 |
| 1 | -1.36792513 | -4.07491931 | 3.82676947 |
| 6 | -2.64433265 | -2.55173024 | 2.96752907 |
| 1 | -3.73295403 | -2.35516504 | 2.91155517 |
| 1 | -2.27621535 | -2.80882429 | 1.96697229 |
| 6 | -1.28443537 | 2.65954806 | 4.54979770 |
| 1 | -1.32633025 | 2.09730191 | 5.50125190 |
| 1 | -0.23725461 | 2.92097562 | 4.33756605 |
| 6 | -2.21115207 | 3.87567055 | 4.57271739 |
| 1 | -2.27871090 | 4.33632807 | 5.56949460 |
| 1 | -1.84970501 | 4.64120461 | 3.86749299 |
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| 1 | -4.22503419 | 4.03172428 | 3.66352430 |
| 1 | -4.05705427 | 2.76258751 | 4.90277414 |
| 6 | -3.06036052 | 2.28190243 | 3.02687254 |
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128
Eu_thf_3_2_N2Ph2_2_AV11__Ci__b3lyp__Def2TZV_MWB53
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8        1.76975736     -1.53195447     -3.45088067
7       -0.68074047     -1.69186687      0.08906172
7        0.80899861     -1.61406287      0.04154702
6       -1.31201974     -2.59785936     -0.74049545
6       -0.66311186     -3.57353619     -1.55203163
1        0.41228842     -3.65266721     -1.50255404
6       -1.39641348     -4.44337664     -2.35796860
1       -0.86770874     -5.18820667     -2.94327689
6       -2.79183573     -4.39108538     -2.41365475
1       -3.35064717     -5.07864800     -3.03358737
6       -3.45015247     -3.43531219     -1.62363474
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6        2.94165839     -2.37913055      0.86273839
1        3.37960492     -1.50240740      0.40083962
6        3.73752581     -3.27851962      1.55684834
1        4.80611070     -3.10384941      1.61582373
6        3.18137965     -4.40477715      2.18395388
1        3.80628624     -5.10917042      2.71583931
6        1.80097910     -4.59974203      2.08542821
1        1.35012648     -5.47098797      2.54766717
6        0.98468105     -3.70713299      1.39213835
1       -0.07403909     -3.89717853      1.30821484
6       -2.29328466     -0.78078143     -4.13678747
1       -2.25190427     -1.55458650     -3.37666391
1       -1.98478814     -1.19079991     -5.10242169
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1       -4.05430231      0.06562735     -3.23292484
1       -4.35538692     -0.61145963     -4.83983101
6       -3.25521391      1.30161278     -4.84477515
1       -3.95322645      2.08876491     -4.56684637
1       -3.23456842      1.23266286     -5.93397323
6       -1.84623781      1.58462817     -4.28858667
1       -1.15184980      1.92213025     -5.05833400
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1        2.25997183     -4.10878563     -5.49124251
1        1.80014301     -4.40273565     -3.81100714
6        3.51747218     -3.08071295     -3.99835572
1        4.15857457     -3.84641783     -3.56386135
1        4.06130629     -2.60047120     -4.81442952
6        3.07402808     -2.04789675     -2.95941277
1        2.91385201     -2.49239767     -1.97816420
1        3.74634726     -1.19649852     -2.86865328
63      -0.41241616      0.12900247      1.81596132
8        1.36386273     -0.03155916      3.80879869
8       -2.07116313     -1.34419424      3.30496552
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7        0.70194359      1.94819500     -0.02678047
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| 1 | -0.39108529 | 3.90899534 | 1.56483529 |
| 6 | 1.41761661 | 4.69970477 | 2.42024985 |
| 1 | 0.88891186 | 5.44453479 | 3.00555814 |
| 6 | 2.81303886 | 4.64741350 | 2.47593600 |
| 1 | 3.37185030 | 5.33497612 | 3.09586862 |
| 6 | 3.47135560 | 3.69164032 | 1.68591599 |
| 1 | 4.55356447 | 3.63097402 | 1.70777991 |
| 6 | 2.76064419 | 2.81644419 | 0.87843408 |
| 1 | 3.28007597 | 2.07490831 | 0.28386804 |
| 6 | -1.50764492 | 2.81592617 | -0.68482389 |
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| 6 | -1.77977598 | 4.85607015 | -2.02314696 |
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| 6 | 2.31448778 | 1.03710956 | 4.19906872 |
| 1 | 2.27310740 | 1.81091462 | 3.43894516 |
| 1 | 2.00599126 | 1.44712804 | 5.16470294 |
| 6 | 3.65747674 | 0.32062354 | 4.29344991 |
| 1 | 4.07550543 | 0.19070078 | 3.29520609 |
| 1 | 4.37659005 | 0.86778776 | 4.90211226 |
| 6 | 3.27641704 | -1.04528466 | 4.90705640 |
| 1 | 3.97442957 | -1.83243679 | 4.62912762 |
| 1 | 3.25577154 | -0.97633473 | 5.99625448 |
| 6 | 1.86744094 | -1.32830004 | 4.35086792 |
| 1 | 1.17305292 | -1.66580213 | 5.12061525 |
| 1 | 1.87547210 | -2.03757705 | 3.52923440 |
| 6 | -2.20688163 | -1.21775173 | 4.77513177 |
| 1 | -1.23863882 | -0.89888347 | 5.15578879 |
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| 1 | -3.69252854 | -2.61183061 | 5.55354017 |
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| 6 | -2.37904899 | -3.55409504 | 4.09293538 |
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| 1 | -1.27764179 | 2.14149934 | 5.52247888 |
| 1 | -0.19997814 | 2.92275025 | 4.33668026 |
| 6 | -2.15528684 | 3.90772869 | 4.56819428 |
| 1 | -2.23876870 | 4.36511376 | 5.55352376 |
| 1 | -1.77893988 | 4.65906377 | 3.87328839 |
| 6 | -3.49626905 | 3.33704108 | 4.06063697 |
| 1 | -4.13737144 | 4.10274595 | 3.62614260 |
| 1 | -4.04010316 | 2.85679932 | 4.87671077 |
| 6 | -3.05282495 | 2.30422487 | 3.02169402 |
| 1 | -2.89264889 | 2.74872579 | 2.04044545 |
| 1 | -3.72514413 | 1.45282665 | 2.93093453 |

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128
Eu_thf_3_2_N2Ph2_2_AV11__Ci__camb3lyp_GD3BJ_Def2SVP_MWB53
63       0.38195448       0.10772993      -1.73377825
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8        1.72002717      -1.51793747      -3.34269233
7       -0.66743955      -1.65149971       0.10030087
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6       -1.28776455      -2.47297144      -0.77953965
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6        2.85099425      -2.31995056       0.98928637
1        3.31841676      -1.45107898       0.51837583
6        3.60379141      -3.19956966       1.74780270
1        4.67779648      -3.02230435       1.85716780
6        3.01373251      -4.30054016       2.38136496
1        3.61165656      -4.99136232       2.97796139
6        1.64434242      -4.49768845       2.21163890
1        1.16132479      -5.36059402       2.67986338
6        0.86954607      -3.62986331       1.44764587
1       -0.19191685      -3.82349369       1.30438836
6       -2.13313022      -0.71188944      -4.08457715
1       -1.96564447      -1.52663970      -3.36960759
1       -1.97581747      -1.09866545      -5.10815091
6       -3.47937761      -0.02966119      -3.94580290
1       -3.71604990       0.08818257      -2.87780579
1       -4.29387338      -0.59305427      -4.42067622
6       -3.20979150       1.32798632      -4.59923470
1       -3.84614595       2.12940357      -4.20474100
1       -3.36974592       1.26688322      -5.68632507
6       -1.73139510       1.58732476      -4.28254454
1       -1.16348742       1.91237320      -5.16962842
1       -1.59788487       2.33182869      -3.48711817
6        2.05229971       1.38682236      -4.60029781
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1        2.91565457       0.77834487      -4.91569297
6        2.11381861       2.81852277      -5.16316521
1        1.33889625       2.99854629      -5.92090745
1        3.08789497       3.00284894      -5.63941265
6        1.94337192       3.70479144      -3.92300834
1        2.46065971       4.67024557      -4.00759941
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6        2.09715473      -3.60842579      -4.34232767
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1        1.60803710      -4.31978906      -3.66025314
6        3.40671759      -3.10823666      -3.73490273
1        3.98973218      -3.89689389      -3.24068284
1        4.03991416      -2.64938225      -4.51050307
6        2.91276410      -2.05587032      -2.75294698
1        2.65988387      -2.48853228      -1.77272587
1        3.62428193      -1.23088560      -2.59708398
63      -0.36075184       0.14860840       1.79605383
8        1.21616857      -0.07865634       3.87873482
8       -2.03258911      -1.26040125       3.23959113
8       -1.69883805       1.77427960       3.40495748
7        0.68866070       1.90783052      -0.03801915
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7      -0.74235820      1.84462100     -0.01322934
6       1.30899350      2.72928828      0.84182976
6       0.64991676      3.65275149      1.69917966
1      -0.42967114      3.76403343      1.60890909
6       1.36925173      4.43297016      2.60067493
1       0.82736712      5.14179225      3.23460644
6       2.75580944      4.34463652      2.70390077
1       3.30783278      4.96643269      3.41035120
6       3.42350089      3.44963983      1.85709632
1       4.51236612      3.36245768      1.91144295
6       2.73001580      2.66092288      0.95715065
1       3.25995017      1.95379091      0.31390518
6      -1.42687087      2.75625338     -0.74800114
6      -2.82977195      2.57632200     -0.92698767
1      -3.29720749      1.70746462     -0.45606328
6      -3.58256026      3.45596005     -1.68548983
1      -4.65657154      3.27872101     -1.79483403
6      -2.99248531      4.55691351     -2.31906811
1      -3.59040250      5.24774673     -2.91565751
6      -1.62308696      4.75402679     -2.14937024
1      -1.14005526      5.61691719     -2.61760863
6      -0.84829937      3.88618849     -1.38538323
1       0.21317282      4.07979072     -1.24214677
6       2.15435141      0.96821703      4.14682876
1       1.98687054      1.78295975      3.43184783
1       1.99705691      1.35501080      5.17039829
6       3.50058536      0.28596450      4.00804639
1       3.73724416      0.16810528      2.94004838
1       4.31509577      0.84935152      4.48290302
6       3.23098751     -1.07167092      4.66149794
1       3.86732447     -1.87310280      4.26700451
1       3.39095645     -1.01055722      5.74858504
6       1.75258323     -1.33099021      4.34483056
1       1.18468124     -1.65602068      5.23192369
1       1.61905149     -2.07549915      3.54941386
6      -2.03111375     -1.13046559      4.66257345
1      -1.11524909     -0.59271675      4.94442723
1      -2.89446743     -0.52197870      4.97795479
6      -2.09264735     -2.56215794      5.22545760
1      -1.31773383     -2.74217604      5.98321031
1      -3.06673049     -2.74647209      5.70169557
6      -1.92219372     -3.44844169      3.98531212
1      -2.43948635     -4.41389220      4.06991146
1      -0.85927837     -3.64459541      3.78105478
6      -2.48707005     -2.56721597      2.88621418
1      -3.59253382     -2.58569795      2.87614510
1      -2.11245492     -2.77981303      1.87817532
6      -1.25705783      2.58457967      4.49476727
1      -1.44405570      2.04489588      5.44011929
1      -0.17758983      2.75819486      4.39238938
6      -2.07601321      3.86477620      4.40455773
1      -2.20096124      4.35612414      5.37912450
1      -1.58692841      4.57614185      3.72246343
6      -3.38557029      3.36453650      3.79716034
1      -3.96861519      4.15316585      3.30293286
1      -4.01874202      2.90567845      4.57277971
6      -2.89159810      2.31216544      2.81521881
1      -2.63874789      2.74481369      1.83498444
1      -3.60309407      1.48715673      2.65938345
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128
Eu_thf_3_2_N2Ph2_2_AV11__Ci__camb3lyp_GD3BJ_Def2TZV_MWB53
63       0.44944044       0.11690446      -1.71454528
8       -1.17249229       0.32979315      -3.73907573
8        2.11875679       1.51082910      -3.12160933
8        1.71705802      -1.51410436      -3.33703661
7       -0.69210074      -1.67376937       0.08959497
7        0.78398061      -1.60354084       0.07291281
6       -1.30151689      -2.52983984      -0.78877466
6       -0.63117942      -3.45066097      -1.63047454
1        0.44076500      -3.53307995      -1.54756571
6       -1.33824385      -4.25282435      -2.51534354
1       -0.79612740      -4.95728635      -3.13462575
6       -2.72384882      -4.18447937      -2.61323738
1       -3.26378477      -4.81969959      -3.29961305
6       -3.40260379      -3.29003685      -1.78016719
1       -4.48179404      -3.22320473      -1.83235734
6       -2.71870669      -2.48212561      -0.89555070
1       -3.24730248      -1.77951414      -0.26520416
6        1.46692652      -2.54701042       0.79562422
6        2.86565994      -2.37084817       0.97317382
1        3.32326390      -1.49672069       0.52864312
6        3.61814470      -3.26662063       1.70537487
1        4.68211236      -3.09784354       1.81585232
6        3.02703915      -4.37873570       2.31111523
1        3.61982716      -5.07907154       2.88079425
6        1.65982486      -4.57124652       2.14230308
1        1.18382855      -5.43694554       2.58590906
6        0.88735423      -3.68547286       1.40414048
1       -0.16497261      -3.86796704       1.26143806
6       -2.13744720      -0.73648594      -4.04147450
1       -1.98521993      -1.53948855      -3.32987933
1       -1.95567666      -1.10104308      -5.05434358
6       -3.47963123      -0.03974109      -3.92131111
1       -3.73999828       0.06037640      -2.86889961
1       -4.27581336      -0.58164155      -4.42617504
6       -3.20383182       1.33803107      -4.54697686
1       -3.84397149       2.11329115      -4.13734084
1       -3.35661134       1.29953620      -5.62534887
6       -1.72976675       1.61261604      -4.21700626
1       -1.15695564       1.92840568      -5.08764799
1       -1.60851619       2.33592480      -3.41845211
6        2.09755517       1.38321357      -4.58413641
1        1.18366982       0.85501587      -4.83988193
1        2.95008051       0.78155373      -4.89287863
6        2.14973834       2.81933286      -5.13659749
1        1.38769997       2.98956669      -5.89389898
1        3.11992196       3.01862658      -5.58999339
6        1.94462976       3.71339411      -3.89860009
1        2.43263897       4.68041353      -3.99699512
1        0.88511146       3.87872781      -3.71009748
6        2.52979049       2.87497497      -2.77471790
1        3.62015406       2.92201316      -2.75185787
1        2.12730041       3.07446614      -1.78876950
6        1.25747353      -2.37773584      -4.42806030
1        1.44379549      -1.86346827      -5.37184832
1        0.19178477      -2.53748913      -4.30095406
6        2.07942253      -3.65558589      -4.29976738
1        2.21302119      -4.15751653      -5.25540746
1        1.59122538      -4.34625883      -3.61417992
6        3.40164306      -3.15846595      -3.69771372
1        3.94861073      -3.94566037      -3.18470161
1        4.04253148      -2.74566027      -4.47722362
6        2.94589721      -2.06559885      -2.73808182
1        2.69218092      -2.45625393      -1.75542381
1        3.65370381      -1.24693165      -2.63340344
63      -0.42823828       0.13941789       1.77682037
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7        0.71329563       1.93009752      -0.02732148
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6       3.42378078      3.54637600      1.84245562
1       4.50297177      3.47955483      1.89464902
6       2.73989531      2.73846641      0.95782973
1       3.26849878      2.03586227      0.32748110
6      -1.44573612      2.80333902     -0.73333554
6      -2.84447296      2.62717818     -0.91086697
1      -3.30206695      1.75303937     -0.46634892
6      -3.59697401      3.52297005     -1.64302791
1      -4.66094317      3.35419449     -1.75348925
6      -3.00588142      4.63510317     -2.24874833
1      -3.59868089      5.33545479     -2.81839552
6      -1.63866375      4.82761162     -2.07995638
1      -1.16267838      5.69332485     -2.52354560
6      -0.86617779      3.94181849     -1.34183286
1       0.18614970      4.12431491     -1.19913841
6       2.15864464      0.99279818      4.10374751
1       2.00639057      1.79581532      3.39217369
1       1.97688941      1.35733051      5.11662843
6       3.50083727      0.29607681      3.98353934
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6       1.75100379     -1.35631409      4.27922753
1       1.17821504     -1.67213905      5.14987158
1       1.62975178     -2.07960235      3.48065293
6      -2.07635540     -1.12688420      4.64640775
1      -1.16247115     -0.59868548      4.90215134
1      -2.92888073     -0.52522435      4.95514997
6      -2.12853649     -2.56300248      5.19887178
1      -1.36650215     -2.73323157      5.95617755
1      -3.09872222     -2.76229913      5.65226168
6      -1.92341775     -3.45706545      3.96087698
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1      -0.86389765     -3.62239016      3.77237754
6      -2.50858334     -2.61865244      2.83699282
1      -3.59894570     -2.66569853      2.81413055
1      -2.10608915     -2.81814451      1.85104624
6      -1.23624785      2.63403451      4.49035397
1      -1.42258280      2.11976063      5.43413629
1      -0.17055621      2.79377068      4.36325521
6      -2.05817507      3.91189815      4.36206761
1      -2.19177045      4.41382383      5.31771045
1      -1.56996358      4.60256842      3.67648658
6      -3.38040082      3.41480330      3.76000475
1      -3.92735474      4.20201008      3.24699746
1      -4.02129959      3.00200043      4.53950809
6      -2.92466828      2.32193693      2.80036534
1      -2.67094103      2.71259827      1.81771209
1      -3.63248564      1.50328064      2.69567661
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128
Eu_thf_3_2_N2Ph2_2_AV11__Ci__camb3lyp__Def2SVP_MWB53
63       0.35832216       0.10469878      -1.74591026
8       -1.33535444       0.29011064      -3.79089190
8        2.03055996       1.54290223      -3.23977460
8        1.71796877      -1.51994836      -3.41940567
7       -0.65948138      -1.65642418       0.09444038
7        0.77335473      -1.59788572       0.06636207
6       -1.28229910      -2.51009504      -0.75763857
6       -0.62641005      -3.45924143      -1.59053083
1        0.45587999      -3.55833313      -1.51429738
6       -1.34931304      -4.28638197      -2.44731968
1       -0.80663492      -5.01579886      -3.05723190
6       -2.73857747      -4.22287188      -2.53117926
1       -3.29351660      -4.88408058      -3.19890354
6       -3.40344885      -3.29876321      -1.71461724
1       -4.49452835      -3.22850447      -1.75298302
6       -2.70593269      -2.46311903      -0.85996306
1       -3.23954077      -1.73960295      -0.23811300
6        1.46146620      -2.51303471       0.79866318
6        2.87245250      -2.35727086       0.94123591
1        3.34480083      -1.50322147       0.44841807
6        3.63197266      -3.24312377       1.68662655
1        4.71183916      -3.08345186       1.76309048
6        3.04312874      -4.33151684       2.34299890
1        3.64660234      -5.03052471       2.92473683
6        1.66644219      -4.50497461       2.21326942
1        1.18222595      -5.35789520       2.69886552
6        0.88421080      -3.62816791       1.46567909
1       -0.18374656      -3.80972721       1.35563215
6       -2.22966978      -0.76320633      -4.16120536
1       -2.11187945      -1.59176303      -3.45095166
1       -1.97994750      -1.12287896      -5.17708185
6       -3.59655597      -0.10539726      -4.12712214
1       -3.93554075      -0.02796450      -3.08339010
1       -4.35286239      -0.66535098      -4.69422709
6       -3.29861568       1.27911819      -4.71143144
1       -3.96334023       2.05973660      -4.32004773
1       -3.40201859       1.26424761      -5.80688998
6       -1.83856016       1.53593013      -4.30768198
1       -1.22148018       1.84449865      -5.16827978
1       -1.74433280       2.29347321      -3.51870556
6        2.09720795       1.42526702      -4.66297332
1        1.12873199       1.03731228      -5.01132016
1        2.87278529       0.69210405      -4.93810713
6        2.41089451       2.83314709      -5.19948325
1        1.75647613       3.11425322      -6.03606144
1        3.44818193       2.88293660      -5.56272627
6        2.23142894       3.73382810      -3.97220084
1        2.85912557       4.63509262      -4.00191569
1        1.18252119       4.04807074      -3.86041772
6        2.59923725       2.79209840      -2.83994359
1        3.69588632       2.68727613      -2.74231722
1        2.17674209       3.04651286      -1.86090110
6        1.25815679      -2.33463530      -4.50067792
1        1.35970491      -1.76819670      -5.44373542
1        0.19711309      -2.57046387      -4.34101597
6        2.15005291      -3.56941283      -4.48876123
1        2.24527242      -4.03129071      -5.48117843
1        1.74119304      -4.32309522      -3.79875064
6        3.46315419      -3.00940426      -3.94436023
1        4.11713007      -3.77429313      -3.50405423
1        4.02484184      -2.49988449      -4.74338498
6        2.96900343      -2.00616611      -2.91069980
1        2.79729433      -2.47537755      -1.92881019
1        3.64541387      -1.14853578      -2.77401247
63      -0.33711904       0.15162935       1.80819151
8        1.35655756      -0.03378251       3.85317315
8       -2.00935684      -1.28657411       3.30205585
8       -1.69676564       1.77627648       3.48168692
7        0.68068450       1.91275230      -0.03215913
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| 7 | -0.75215160 | 1.85421385 | -0.00408082 |
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| 6 | 0.64761317 | 3.71556955 | 1.65281208 |
| 1 | -0.43467687 | 3.81466125 | 1.57657863 |
| 6 | 1.37051616 | 4.54271009 | 2.50960093 |
| 1 | 0.82783804 | 5.27212698 | 3.11951315 |
| 6 | 2.75978059 | 4.47920000 | 2.59346051 |
| 1 | 3.31471973 | 5.14040871 | 3.26118479 |
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| 1 | 4.51573148 | 3.48483260 | 1.81526427 |
| 6 | 2.72713581 | 2.71944716 | 0.92224431 |
| 1 | 3.26074390 | 1.99593108 | 0.30039425 |
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| 1 | -3.32359771 | 1.75954959 | -0.38613682 |
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| 6 | -0.86300767 | 3.88449603 | -1.40339784 |
| 1 | 0.20494969 | 4.06605534 | -1.29335090 |
| 6 | 2.25087290 | 1.01953445 | 4.22348661 |
| 1 | 2.13308258 | 1.84809115 | 3.51323291 |
| 1 | 2.00115063 | 1.37920709 | 5.23936310 |
| 6 | 3.61775910 | 0.36172538 | 4.18940339 |
| 1 | 3.95674387 | 0.28429263 | 3.14567135 |
| 1 | 4.37406552 | 0.92167910 | 4.75650834 |
| 6 | 3.31981880 | -1.02279006 | 4.77371269 |
| 1 | 3.98454335 | -1.80340847 | 4.38232898 |
| 1 | 3.42322172 | -1.00791948 | 5.86917123 |
| 6 | 1.85976329 | -1.27960200 | 4.36996323 |
| 1 | 1.24268330 | -1.58817053 | 5.23056103 |
| 1 | 1.76553592 | -2.03714508 | 3.58098681 |
| 6 | -2.07600482 | -1.16893889 | 4.72525457 |
| 1 | -1.10752887 | -0.78098416 | 5.07360141 |
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| 1 | -1.73527300 | -2.85792510 | 6.09834269 |
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| 1 | -1.16131807 | -3.79174261 | 3.92269897 |
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| 1 | -3.67468320 | -2.43094801 | 2.80459847 |
| 1 | -2.15553896 | -2.79018474 | 1.92318235 |
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| 1 | -1.33850178 | 2.02452482 | 5.50601667 |
| 1 | -0.17590996 | 2.82679199 | 4.40329722 |
| 6 | -2.12884978 | 3.82574095 | 4.55104248 |
| 1 | -2.22406929 | 4.28761884 | 5.54345968 |
| 1 | -1.71998991 | 4.57942334 | 3.86103189 |
| 6 | -3.44195106 | 3.26573238 | 4.00664148 |
| 1 | -4.09592694 | 4.03062126 | 3.56633548 |
| 1 | -4.00363872 | 2.75621261 | 4.80566623 |
| 6 | -2.94780031 | 2.26249423 | 2.97298105 |
| 1 | -2.77609121 | 2.73170568 | 1.99109144 |
| 1 | -3.62421075 | 1.40486391 | 2.83629372 |

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128
Eu_thf_3_2_N2Ph2_2_AV11__Ci__camb3lyp__Def2TZV_MWB53
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8        2.09560380      1.55114973     -3.17469377
8        1.71907553     -1.50721587     -3.41189807
7       -0.67693077     -1.68491853      0.07866958
7        0.80149729     -1.61412085      0.04979728
6       -1.29277236     -2.57566812     -0.76596627
6       -0.62917465     -3.52167607     -1.58656429
1        0.44554233     -3.59046970     -1.52502368
6       -1.34321360     -4.37254932     -2.41989458
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6       -2.73154708     -4.32972909     -2.49027142
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6       -2.71276011     -2.54954090     -0.85206072
1       -3.24185913     -1.82863969     -0.24293920
6        1.49656158     -2.55717190      0.76825573
6        2.90218363     -2.39355817      0.90784729
1        3.35759081     -1.52862634      0.44328869
6        3.66879336     -3.28998981      1.62584930
1        4.73701505     -3.12873950      1.70401664
6        3.08797444     -4.39552515      2.25339733
1        3.69189786     -5.09922802      2.80748810
6        1.71471148     -4.57570326      2.12631410
1        1.24441175     -5.43561695      2.58746285
6        0.92749737     -3.68637998      1.40678851
1       -0.13018275     -3.86431738      1.29919534
6       -2.22712998     -0.77857526     -4.10286124
1       -2.13584218     -1.57532248     -3.37266789
1       -1.95421023     -1.14961756     -5.09313600
6       -3.58209771     -0.09279571     -4.11358172
1       -3.94882062      0.00275558     -3.09291517
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6       -3.26052537      1.28896843     -4.70812232
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6        2.17875449      1.42416217     -4.63617536
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1        1.87780249      3.09620726     -6.02066435
6        2.26372549      3.75669545     -3.96153224
1        2.87019183      4.65879684     -4.00166773
1        1.21591908      4.04713516     -3.89451697
6        2.62119549      2.86532516     -2.78382674
1        3.70162533      2.78840872     -2.64628856
1        2.14863550      3.12032796     -1.84294055
6        1.23112552     -2.37932987     -4.48765496
1        1.33257846     -1.84301516     -5.43217643
1        0.18394943     -2.59209519     -4.29692360
6        2.11751404     -3.62039180     -4.43655022
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1        1.70005362     -4.35052413     -3.74454043
6        3.44703518     -3.07606348     -3.89420646
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1        4.02521546     -2.61591447     -4.69621798
6        2.99395118     -2.02731759     -2.88423068
1        2.80246147     -2.45497611     -1.90227791
1        3.67552932     -1.18545450     -2.78779407
63      -0.40600939      0.13143280      1.79367817
8        1.31773571     -0.03855897      3.78635649
8       -2.07440067     -1.29482161      3.23697502
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7        0.69813389      1.94124666     -0.01638833
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| 1 | -0.42433920 | 3.84679782 | 1.58730493 |
| 6 | 1.36441673 | 4.62887745 | 2.48217583 |
| 1 | 0.82395153 | 5.35333242 | 3.07999095 |
| 6 | 2.75275020 | 4.58605721 | 2.55255267 |
| 1 | 3.29805052 | 5.26079854 | 3.19603884 |
| 6 | 3.42524955 | 3.66187814 | 1.74797271 |
| 1 | 4.50646652 | 3.61139909 | 1.77904097 |
| 6 | 2.73396324 | 2.80586903 | 0.91434197 |
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| 6 | -1.47535846 | 2.81350003 | -0.70597448 |
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| 6 | -0.90629424 | 3.94270811 | -1.34450726 |
| 1 | 0.15138588 | 4.12064550 | -1.23691409 |
| 6 | 2.24833310 | 1.03490338 | 4.16514249 |
| 1 | 2.15704530 | 1.83165060 | 3.43494914 |
| 1 | 1.97541335 | 1.40594568 | 5.15541725 |
| 6 | 3.60330084 | 0.34912383 | 4.17586297 |
| 1 | 3.97002374 | 0.25357255 | 3.15519642 |
| 1 | 4.34031800 | 0.89671194 | 4.75916864 |
| 6 | 3.28172850 | -1.03264030 | 4.77040357 |
| 1 | 3.96737869 | -1.80106798 | 4.42401427 |
| 1 | 3.33223976 | -0.99551118 | 5.85856687 |
| 6 | 1.84763228 | -1.32012200 | 4.30209839 |
| 1 | 1.20281315 | -1.65332130 | 5.11414974 |
| 1 | 1.80918008 | -2.03668332 | 3.48907789 |
| 6 | -2.15755137 | -1.16783404 | 4.69845661 |
| 1 | -1.19722579 | -0.78949987 | 5.03907878 |
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| 1 | -1.85659936 | -2.83987913 | 6.08294560 |
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| 1 | -1.19471596 | -3.79080704 | 3.95679822 |
| 6 | -2.59999237 | -2.60899703 | 2.84610799 |
| 1 | -3.68042221 | -2.53208059 | 2.70856981 |
| 1 | -2.12743238 | -2.86399984 | 1.90522180 |
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| 1 | -4.03607912 | 4.10478447 | 3.49442503 |
| 1 | -4.00401234 | 2.87224259 | 4.75849923 |
| 6 | -2.97274805 | 2.28364571 | 2.94651193 |
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128
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63       0.35003640       0.12767610      -1.74211998
8       -1.23112648       0.23811699      -3.84892280
8        2.04340948       1.58522613      -3.13316675
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7       -0.70355533      -1.60104524       0.04340557
7        0.72084702      -1.58628294       0.04290524
6       -1.32011744      -2.46171508      -0.79778026
6       -0.65366529      -3.42805055      -1.59322250
1        0.42560495      -3.53462313      -1.47929763
6       -1.36160496      -4.24760551      -2.46422499
1       -0.81379233      -4.98905580      -3.05432407
6       -2.74359099      -4.15926595      -2.59335162
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6       -2.73534507      -2.39260697      -0.93709604
1       -3.27041520      -1.64643461      -0.34350985
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6        2.75342398      -2.35415639       1.04409838
1        3.27607941      -1.55285292       0.51463442
6        3.44329081      -3.21825166       1.87136350
1        4.52583266      -3.10006614       1.97802058
6        2.78398607      -4.22906829       2.57856208
1        3.33466707      -4.90850879       3.23141808
6        1.40891182      -4.35244313       2.41058400
1        0.87047970      -5.14542615       2.93896414
6        0.69539577      -3.50182538       1.57470646
1       -0.37474994      -3.64118141       1.42555678
6       -2.12771313      -0.84918676      -4.05762102
1       -1.88108011      -1.65369745      -3.35243993
1       -2.01658875      -1.23360800      -5.08748553
6       -3.48969350      -0.23138304      -3.83775936
1       -3.65893759      -0.11226881      -2.75784404
1       -4.30578359      -0.83937919      -4.24849803
6       -3.32666602       1.12224013      -4.51995970
1       -3.96654110       1.90158396      -4.08965438
1       -3.56332419       1.04210387      -5.59084886
6       -1.84528364       1.44449150      -4.31651523
1       -1.35828289       1.75903143      -5.25329608
1       -1.68632218       2.22511243      -3.55973473
6        1.88252640       1.72795391      -4.53095876
1        1.09369684       1.03773837      -4.85814689
1        2.82140592       1.45843803      -5.04914199
6        1.54837010       3.19871602      -4.70472227
1        0.48543934       3.36180111      -4.47972289
1        1.74499300       3.56424186      -5.72121673
6        2.42315661       3.86631134      -3.64079047
1        3.34947410       4.26371130      -4.07774748
1        1.90493609       4.70226362      -3.15445976
6        2.73274518       2.73486615      -2.65105322
1        3.81295164       2.51650080      -2.61188588
1        2.37618714       2.91988604      -1.63103318
6        1.25554737      -2.37130349      -4.39253336
1        1.42901362      -1.84860751      -5.34868932
1        0.18069190      -2.57007333      -4.28788159
6        2.09874420      -3.62940630      -4.27645519
1        2.24562209      -4.12939375      -5.24264453
1        1.61724827      -4.34290406      -3.59237027
6        3.38413853      -3.09682099      -3.66000087
1        3.97817433      -3.86670404      -3.15113992
1        4.01630533      -2.62771598      -4.42906377
6        2.84946386      -2.05363265      -2.69805886
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1        3.54667808      -1.22219400      -2.51748509
63      -0.32883327       0.12865203       1.80440123
8        1.25232960       0.01821113       3.91120405
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7        0.72475846       1.85737337       0.01887568
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| 6 | 1.38280809 | 4.50393363 | 2.52650624 |
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| 6 | 2.76479412 | 4.41559407 | 2.65563287 |
| 1 | 3.30887687 | 5.06968450 | 3.33909932 |
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| 1 | 4.52667163 | 3.38857552 | 1.94271477 |
| 6 | 2.75654819 | 2.64893509 | 0.99937729 |
| 1 | 3.29161832 | 1.90276274 | 0.40579110 |
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| 1 | 0.39595306 | 3.89750953 | -1.36327553 |
| 6 | 2.14891626 | 1.10551488 | 4.11990227 |
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| 1 | 2.03779188 | 1.48993612 | 5.14976678 |
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| 1 | 3.68014071 | 0.36859693 | 2.82012529 |
| 1 | 4.32698671 | 1.09570731 | 4.31077928 |
| 6 | 3.34786915 | -0.86591200 | 4.58224095 |
| 1 | 3.98774422 | -1.64525583 | 4.15193563 |
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| 6 | 1.86648676 | -1.18816338 | 4.37879648 |
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| 1 | -2.22441896 | 4.38572188 | 5.30492578 |
| 1 | -1.59604514 | 4.59923219 | 3.65465152 |
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| 1 | -3.95697120 | 4.12303216 | 3.21342117 |
| 1 | -3.99510220 | 2.88404411 | 4.49134502 |
| 6 | -2.82826074 | 2.30996078 | 2.76034011 |
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128
Eu_thf_3_2_N2Ph2_2_AV11__Ci__lcwpbe_GD3BJ_Def2TZV_MWB53
63       0.42737443       0.13085831      -1.71308234
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7       -0.70966358      -1.62335206       0.02727130
7        0.75456005      -1.60192322       0.04977596
6       -1.30900569      -2.52451602      -0.80845511
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1        0.44499303      -3.57954944      -1.45090223
6       -1.31523842      -4.34404882      -2.42178916
1       -0.76260524      -5.08926136      -2.98347681
6       -2.69407683      -4.27002452      -2.56249697
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1       -4.46248780      -3.24886876      -1.89392295
6       -2.71759950      -2.47058143      -0.95555162
1       -3.25369104      -1.71950549      -0.38841867
6        1.37366481      -2.52602913       0.84469879
6        2.77602732      -2.42722318       1.02666406
1        3.29308294      -1.61950854       0.52282737
6        3.46037024      -3.31496779       1.82652509
1        4.53449338      -3.21299399       1.93265366
6        2.79340293      -4.33478358       2.50607783
1        3.33553286      -5.03082638       3.13125894
6        1.42007222      -4.44457574       2.34069201
1        0.88332047      -5.24077108       2.84461335
6        0.71487839      -3.56846043       1.53122993
1       -0.34780483      -3.68975076       1.38584132
6       -2.11182947      -0.85597092      -4.01408268
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1       -1.96066509      -1.19040837      -5.04323242
6       -3.48738708      -0.26060210      -3.81100244
1       -3.68764289      -0.18678916      -2.74287768
1       -4.27201627      -0.85719419      -4.27116540
6       -3.34525984       1.13047402      -4.43604226
1       -3.99303611       1.86389611      -3.96382650
1       -3.58536340       1.09515695      -5.49895873
6       -1.87103878       1.48688579      -4.22649022
1       -1.38459502       1.79020245      -5.15347350
1       -1.72960492       2.25578848      -3.47250528
6        1.95681127       1.68069483      -4.48597237
1        1.18745504       0.96986758      -4.77467601
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6        1.56237519       3.14005623      -4.62017426
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1        1.68655143       3.51881956      -5.63296863
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1        2.00280906       4.70558608      -3.16250129
6        2.78501515       2.75989682      -2.56131290
1        3.85522547       2.59510682      -2.43686352
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1        0.14488779      -2.67152809      -4.23660519
6        2.08140265      -3.68730307      -4.23561335
1        2.22819903      -4.21009258      -5.17863854
1        1.63548416      -4.38006769      -3.52250108
6        3.37657448      -3.10991127      -3.66552845
1        3.97295523      -3.85480239      -3.14313794
1        3.98303783      -2.67430757      -4.46075841
6        2.86638048      -2.03134214      -2.72663597
1        2.61505770      -2.42756290      -1.74322245
1        3.53959685      -1.18334374      -2.61935490
63      -0.40617130       0.12546981       1.77536359
8        1.24153500      -0.00994591       3.80224420
8       -2.15958624      -1.26847925       3.12214298
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7        0.73086670       1.87968019       0.03500995
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| 6 | 2.71527996 | 4.52635265 | 2.62477822 |
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| 1 | 4.48369093 | 3.50519688 | 1.95620420 |
| 6 | 2.73880263 | 2.72690955 | 1.01783287 |
| 1 | 3.27489417 | 1.97583362 | 0.45069992 |
| 6 | -1.35246169 | 2.78235726 | -0.78241754 |
| 6 | -2.75482419 | 2.68355131 | -0.96438281 |
| 1 | -3.27187982 | 1.87583666 | -0.46054612 |
| 6 | -3.43916711 | 3.57129592 | -1.76424384 |
| 1 | -4.51329025 | 3.46932212 | -1.87037241 |
| 6 | -2.77219980 | 4.59111170 | -2.44379658 |
| 1 | -3.31432974 | 5.28715451 | -3.06897769 |
| 6 | -1.39886909 | 4.70090387 | -2.27841076 |
| 1 | -0.86211734 | 5.49709921 | -2.78233210 |
| 6 | -0.69367527 | 3.82478855 | -1.46894868 |
| 1 | 0.36900795 | 3.94607888 | -1.32356007 |
| 6 | 2.13303260 | 1.11229904 | 4.07636393 |
| 1 | 1.89124655 | 1.91693951 | 3.38870963 |
| 1 | 1.98186821 | 1.44673650 | 5.10551367 |
| 6 | 3.50859020 | 0.51693022 | 3.87328369 |
| 1 | 3.70884602 | 0.44311729 | 2.80515893 |
| 1 | 4.29321940 | 1.11352231 | 4.33344665 |
| 6 | 3.36646296 | -0.87414589 | 4.49832351 |
| 1 | 4.01423924 | -1.60756799 | 4.02610775 |
| 1 | 3.60656653 | -0.83882883 | 5.56123998 |
| 6 | 1.89224191 | -1.23055767 | 4.28877147 |
| 1 | 1.40579815 | -1.53387432 | 5.21575475 |
| 1 | 1.75080804 | -1.99946035 | 3.53478653 |
| 6 | -1.93560814 | -1.42436671 | 4.54825362 |
| 1 | -1.16625191 | -0.71353945 | 4.83695726 |
| 1 | -2.85860586 | -1.19990391 | 5.08856820 |
| 6 | -1.54117206 | -2.88372810 | 4.68245551 |
| 1 | -0.50085827 | -3.01009382 | 4.38612684 |
| 1 | -1.66534830 | -3.26249144 | 5.69524988 |
| 6 | -2.46073393 | -3.58127210 | 3.67218035 |
| 1 | -3.37850150 | -3.91624402 | 4.15499694 |
| 1 | -1.98160593 | -4.44925795 | 3.22478254 |
| 6 | -2.76381202 | -2.50356870 | 2.62359415 |
| 1 | -3.83402235 | -2.33877869 | 2.49914477 |
| 1 | -2.31335148 | -2.69430319 | 1.65551314 |
| 6 | -1.17771056 | 2.71479730 | 4.45118285 |
| 1 | -1.31980592 | 2.22642981 | 5.41656703 |
| 1 | -0.12368467 | 2.92785622 | 4.29888644 |
| 6 | -2.06019953 | 3.94363119 | 4.29789460 |
| 1 | -2.20699590 | 4.46642071 | 5.24091979 |
| 1 | -1.61428103 | 4.63639582 | 3.58478233 |
| 6 | -3.35537136 | 3.36623940 | 3.72780970 |
| 1 | -3.95175210 | 4.11113051 | 3.20541919 |
| 1 | -3.96183470 | 2.93063569 | 4.52303966 |
| 6 | -2.84517736 | 2.28767027 | 2.78891722 |
| 1 | -2.59385457 | 2.68389102 | 1.80550370 |
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128
Eu_thf_3_2_N2Ph2_2_AV11__Ci__lcwpbe__Def2SVP_MWB53
63       0.32143837      0.11529976     -1.74995739
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8        1.91842656      1.62257592     -3.27671914
8        1.74080278     -1.52446211     -3.38733698
7       -0.68493545     -1.63024111      0.08005172
7        0.73955623     -1.58522543      0.05174383
6       -1.31050523     -2.48584197     -0.76291458
6       -0.65600034     -3.43206591     -1.59350201
1        0.42813832     -3.52717932     -1.51695834
6       -1.37906931     -4.26295169     -2.44325505
1       -0.83694008     -4.99333102     -3.05271565
6       -2.76577025     -4.20433822     -2.52233106
1       -3.32140893     -4.86960934     -3.18588879
6       -3.42863500     -3.28005777     -1.70798599
1       -4.52020102     -3.21210887     -1.74312242
6       -2.73184189     -2.44104368     -0.86089164
1       -3.26406834     -1.71462064     -0.24045343
6        1.41540272     -2.49423328      0.79861607
6        2.82194966     -2.34230047      0.95983867
1        3.30384221     -1.49155784      0.46961252
6        3.56637496     -3.22679146      1.71696958
1        4.64611628     -3.07133698      1.80616858
6        2.96542542     -4.30669625      2.37090516
1        3.55797260     -5.00605069      2.96393403
6        1.59215798     -4.47240516      2.22571660
1        1.09771671     -5.32024289      2.71035416
6        0.82502697     -3.59782439      1.46443377
1       -0.24332661     -3.77380017      1.33793728
6       -2.26323335     -0.77881148     -4.15764482
1       -2.13998776     -1.60326114     -3.44208312
1       -2.04444389     -1.15448831     -5.17416319
6       -3.61678185     -0.10401808     -4.09954155
1       -3.92698510     -0.00185029     -3.04948306
1       -4.39542249     -0.66249185     -4.63547904
6       -3.31137915      1.25798942     -4.71560688
1       -3.96555770      2.05524599     -4.34139707
1       -3.42254168      1.21663576     -5.80906201
6       -1.85088081      1.50587218     -4.32871599
1       -1.24250498      1.81660126     -5.19364901
1       -1.74778908      2.26482154     -3.54013417
6        2.10032157      1.52629151     -4.67723148
1        1.28016706      0.92243989     -5.08636854
1        3.04987191      1.00363364     -4.88913035
6        2.13191380      2.97047310     -5.19574641
1        1.20400727      3.22730240     -5.72349408
1        2.95919986      3.11383612     -5.90397914
6        2.30208344      3.81797787     -3.92567126
1        3.09393518      4.57298299     -4.01593760
1        1.36710727      4.33785028     -3.67769891
6        2.61197382      2.78644931     -2.85150243
1        3.69507879      2.56917982     -2.80240945
1        2.25577577      3.03930918     -1.84575966
6        1.30729274     -2.33899823     -4.47198659
1        1.43787709     -1.78022473     -5.41515762
1        0.24014847     -2.56803780     -4.34402673
6        2.18669837     -3.57773387     -4.43134056
1        2.31246524     -4.03820845     -5.42016763
1        1.75011872     -4.33015838     -3.75833477
6        3.47861690     -3.03005207     -3.84170630
1        4.11247434     -3.79964946     -3.38242659
1        4.07011076     -2.51813162     -4.61616405
6        2.95082472     -2.03447632     -2.82468320
1        2.72534135     -2.51318389     -1.85821474
1        3.63420840     -1.19167282     -2.64196458
63      -0.30023524      0.14102837      1.81223864
8        1.37226405     -0.00611048      3.88407964
8       -1.89722343     -1.36624780      3.33900039
8       -1.71959965      1.78079023      3.44961823
7        0.70613857      1.88656923     -0.01777047
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| 7 | -0.71835310 | 1.84155355 | 0.01053742 |
| 6 | 1.33170836 | 2.74217010 | 0.82519583 |
| 6 | 0.67720347 | 3.68839404 | 1.65578326 |
| 1 | -0.40693520 | 3.78350745 | 1.57923959 |
| 6 | 1.40027243 | 4.51927981 | 2.50553630 |
| 1 | 0.85814320 | 5.24965915 | 3.11499690 |
| 6 | 2.78697338 | 4.46066634 | 2.58461231 |
| 1 | 3.34261205 | 5.12593746 | 3.24817004 |
| 6 | 3.44983813 | 3.53638589 | 1.77026724 |
| 1 | 4.54140414 | 3.46843700 | 1.80540367 |
| 6 | 2.75304502 | 2.69737181 | 0.92317289 |
| 1 | 3.28527147 | 1.97094876 | 0.30273468 |
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| 1 | -3.28263908 | 1.74788596 | -0.40733127 |
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| 6 | -1.57095485 | 4.72873329 | -2.16343535 |
| 1 | -1.07651359 | 5.57657101 | -2.64807291 |
| 6 | -0.80382384 | 3.85415251 | -1.40215252 |
| 1 | 0.26452974 | 4.03012830 | -1.27565603 |
| 6 | 2.28443647 | 1.03513961 | 4.21992607 |
| 1 | 2.16119089 | 1.85958926 | 3.50436437 |
| 1 | 2.06564701 | 1.41081643 | 5.23644444 |
| 6 | 3.63798497 | 0.36034621 | 4.16182280 |
| 1 | 3.94818822 | 0.25817841 | 3.11176431 |
| 1 | 4.41662562 | 0.91881997 | 4.69776029 |
| 6 | 3.33258228 | -1.00166129 | 4.77788813 |
| 1 | 3.98676082 | -1.79891786 | 4.40367832 |
| 1 | 3.44374481 | -0.96030763 | 5.87134326 |
| 6 | 1.87208393 | -1.24954405 | 4.39099724 |
| 1 | 1.26370811 | -1.56027314 | 5.25593026 |
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| 6 | -2.11071067 | -2.71414497 | 5.25802766 |
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| 1 | -2.93799673 | -2.85750799 | 5.96626039 |
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| 1 | -3.07273205 | -4.31665487 | 4.07821885 |
| 1 | -1.34590414 | -4.08152216 | 3.73998016 |
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| 6 | -1.28608961 | 2.59532636 | 4.53426784 |
| 1 | -1.41667397 | 2.03655285 | 5.47743887 |
| 1 | -0.21894535 | 2.82436593 | 4.40630798 |
| 6 | -2.16549525 | 3.83406199 | 4.49362181 |
| 1 | -2.29126211 | 4.29453658 | 5.48244888 |
| 1 | -1.72891560 | 4.58648650 | 3.82061602 |
| 6 | -3.45741378 | 3.28638020 | 3.90398755 |
| 1 | -4.09127121 | 4.05597759 | 3.44470784 |
| 1 | -4.04890763 | 2.77445975 | 4.67844530 |
| 6 | -2.92962160 | 2.29080444 | 2.88696445 |
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128
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63       0.35003640       0.12767610      -1.74211998
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8        2.04340948       1.58522613      -3.13316675
8        1.67815007      -1.52985262      -3.32560572
7       -0.70355533      -1.60104524       0.04340557
7        0.72084702      -1.58628294       0.04290524
6       -1.32011744      -2.46171508      -0.79778026
6       -0.65366529      -3.42805055      -1.59322250
1        0.42560495      -3.53462313      -1.47929763
6       -1.36160496      -4.24760551      -2.46422499
1       -0.81379233      -4.98905580      -3.05432407
6       -2.74359099      -4.15926595      -2.59335162
1       -3.28767374      -4.81335637      -3.27681807
6       -3.41795054      -3.22237790      -1.80413614
1       -4.50546850      -3.13224740      -1.88043352
6       -2.73534507      -2.39260697      -0.93709604
1       -3.27041520      -1.64643461      -0.34350985
6        1.34699848      -2.46854145       0.85556196
6        2.75342398      -2.35415639       1.04409838
1        3.27607941      -1.55285292       0.51463442
6        3.44329081      -3.21825166       1.87136350
1        4.52583266      -3.10006614       1.97802058
6        2.78398607      -4.22906829       2.57856208
1        3.33466707      -4.90850879       3.23141808
6        1.40891182      -4.35244313       2.41058400
1        0.87047970      -5.14542615       2.93896414
6        0.69539577      -3.50182538       1.57470646
1       -0.37474994      -3.64118141       1.42555678
6       -2.12771313      -0.84918676      -4.05762102
1       -1.88108011      -1.65369745      -3.35243993
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1       -3.65893759      -0.11226881      -2.75784404
1       -4.30578359      -0.83937919      -4.24849803
6       -3.32666602       1.12224013      -4.51995970
1       -3.96654110       1.90158396      -4.08965438
1       -3.56332419       1.04210387      -5.59084886
6       -1.84528364       1.44449150      -4.31651523
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1       -1.68632218       2.22511243      -3.55973473
6        1.88252640       1.72795391      -4.53095876
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6        1.54837010       3.19871602      -4.70472227
1        0.48543934       3.36180111      -4.47972289
1        1.74499300       3.56424186      -5.72121673
6        2.42315661       3.86631134      -3.64079047
1        3.34947410       4.26371130      -4.07774748
1        1.90493609       4.70226362      -3.15445976
6        2.73274518       2.73486615      -2.65105322
1        3.81295164       2.51650080      -2.61188588
1        2.37618714       2.91988604      -1.63103318
6        1.25554737      -2.37130349      -4.39253336
1        1.42901362      -1.84860751      -5.34868932
1        0.18069190      -2.57007333      -4.28788159
6        2.09874420      -3.62940630      -4.27645519
1        2.24562209      -4.12939375      -5.24264453
1        1.61724827      -4.34290406      -3.59237027
6        3.38413853      -3.09682099      -3.66000087
1        3.97817433      -3.86670404      -3.15113992
1        4.01630533      -2.62771598      -4.42906377
6        2.84946386      -2.05363265      -2.69805886
1        2.56834689      -2.49066739      -1.72682410
1        3.54667808      -1.22219400      -2.51748509
63      -0.32883327       0.12865203       1.80440123
8        1.25232960       0.01821113       3.91120405
8       -2.02220635      -1.32889801       3.19544800
8       -1.65694695       1.78618075       3.38788697
7        0.72475846       1.85737337       0.01887568
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| 7 | -0.69964389 | 1.84261106 | 0.01937601 |
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| 6 | 1.38280809 | 4.50393363 | 2.52650624 |
| 1 | 0.83499546 | 5.24538392 | 3.11660532 |
| 6 | 2.76479412 | 4.41559407 | 2.65563287 |
| 1 | 3.30887687 | 5.06968450 | 3.33909932 |
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| 6 | 2.75654819 | 2.64893509 | 0.99937729 |
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| 1 | 0.39595306 | 3.89750953 | -1.36327553 |
| 6 | 2.14891626 | 1.10551488 | 4.11990227 |
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| 1 | 2.03779188 | 1.48993612 | 5.14976678 |
| 6 | 3.51089662 | 0.48771117 | 3.90004061 |
| 1 | 3.68014071 | 0.36859693 | 2.82012529 |
| 1 | 4.32698671 | 1.09570731 | 4.31077928 |
| 6 | 3.34786915 | -0.86591200 | 4.58224095 |
| 1 | 3.98774422 | -1.64525583 | 4.15193563 |
| 1 | 3.58452731 | -0.78577574 | 5.65313011 |
| 6 | 1.86648676 | -1.18816338 | 4.37879648 |
| 1 | 1.37948601 | -1.50270331 | 5.31557733 |
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| 1 | -3.32827098 | -4.00738317 | 4.14002873 |
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| 1 | -1.40781050 | 2.10493564 | 5.41097057 |
| 1 | -0.15948878 | 2.82640145 | 4.35016284 |
| 6 | -2.07754108 | 3.88573443 | 4.33873644 |
| 1 | -2.22441896 | 4.38572188 | 5.30492578 |
| 1 | -1.59604514 | 4.59923219 | 3.65465152 |
| 6 | -3.36293540 | 3.35314912 | 3.72228212 |
| 1 | -3.95697120 | 4.12303216 | 3.21342117 |
| 1 | -3.99510220 | 2.88404411 | 4.49134502 |
| 6 | -2.82826074 | 2.30996078 | 2.76034011 |
| 1 | -2.54714377 | 2.74699551 | 1.78910535 |
| 1 | -3.52547495 | 1.47852213 | 2.57976634 |

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128
Eu_thf_3_2_N2Ph2_2_AV11__Ci__wb97xd_Def2SVP_MWB53
63       0.36783064       0.10396828      -1.76834633
8       -1.12426263       0.33719707      -3.91842782
8        2.07539700       1.50896115      -3.18419699
8        1.73415023      -1.52565252      -3.33373956
7       -0.65547831      -1.63650119       0.11834229
7        0.77098347      -1.56381825       0.07466161
6       -1.28409906      -2.42287618      -0.78470375
6       -0.63728311      -3.33306653      -1.66862350
1        0.44255827      -3.46070304      -1.58152263
6       -1.37072530      -4.08243841      -2.58747390
1       -0.84073243      -4.78371266      -3.24037703
6       -2.75737909      -3.97037626      -2.68560626
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6       -3.41191792      -3.08293268      -1.81709960
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6       -2.70544040      -2.32545372      -0.89884400
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6        1.46801888      -2.45711228       0.81836950
6        2.86459296      -2.23690633       1.01245131
1        3.31125819      -1.35480104       0.54359320
6        3.63330830      -3.09751981       1.77920242
1        4.70097867      -2.89080319       1.90162282
6        3.06465562      -4.21492911       2.40787203
1        3.67482504      -4.88937957       3.01145026
6        1.70125360      -4.44970639       2.22449082
1        1.23673338      -5.32507450       2.68890197
6        0.91044326      -3.60158495       1.45165482
1       -0.14544577      -3.82280857       1.29545151
6       -2.09844584      -0.68554535      -4.13326825
1       -1.91947091      -1.49891311      -3.41683642
1       -1.99573202      -1.08988045      -5.15735774
6       -3.42202937       0.03031174      -3.94220402
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1        1.19006827       0.77547478      -4.87767079
1        2.97113023       0.83575968      -4.92973731
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1        2.96770686       3.06983754      -5.65649264
6        1.79510713       3.68159484      -3.92351934
1        2.23475394       4.68447928      -4.01217356
1        0.72259585       3.79482272      -3.70194683
6        2.44235796       2.84122742      -2.83582400
1        3.54401493       2.93986287      -2.84365247
1        2.06858771       3.02526322      -1.82031301
6        1.27463827      -2.33023738      -4.41549298
1        1.48437575      -1.80644542      -5.36557381
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1        1.53027005      -4.32890479      -3.62583793
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1        3.63040071      -1.29362026      -2.55967127
63      -0.34662752       0.15235984       1.83062758
8        1.14546576      -0.08086895       3.98070907
8       -2.05419388      -1.25263303       3.24647824
8       -1.71294711       1.78198065       3.39602081
7        0.67668143       1.89282932      -0.05606104
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| 6 | 2.77858221 | 4.22670439 | 2.74788751 |
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| 1 | 0.16664890 | 4.07913670 | -1.23317026 |
| 6 | 2.11964896 | 0.94187347 | 4.19554950 |
| 1 | 1.94067403 | 1.75524124 | 3.47911767 |
| 1 | 2.01693514 | 1.34620857 | 5.21963899 |
| 6 | 3.44323249 | 0.22601639 | 4.00448527 |
| 1 | 3.62952034 | 0.08746245 | 2.92788713 |
| 1 | 4.29131706 | 0.77395605 | 4.43668456 |
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| 1 | -2.94650373 | -2.81350942 | 5.71877389 |
| 6 | -1.77390400 | -3.42526672 | 3.98580059 |
| 1 | -2.21355081 | -4.42815115 | 4.07445481 |
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| 6 | -2.87426056 | 2.35301305 | 2.78348974 |
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128
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8        2.14191866      1.51954727     -3.14322687
8        1.77297586     -1.52949452     -3.31685031
7       -0.69790438     -1.66032311      0.11694180
7        0.77207989     -1.57684081      0.08434138
6       -1.31148827     -2.47465281     -0.79497179
6       -0.64824210     -3.36580993     -1.67851421
1        0.42590970     -3.45697006     -1.60319429
6       -1.36676325     -4.13089440     -2.59100358
1       -0.83200666     -4.81428888     -3.24169079
6       -2.75428916     -4.04990256     -2.67885739
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6        1.46814741     -2.51017920      0.80776067
6        2.86193378     -2.29671005      1.00051843
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6        3.63153175     -3.18022287      1.73381395
1        4.69052357     -2.98417540      1.85744410
6        3.06162285     -4.31308410      2.32756870
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6        1.69964867     -4.54151216      2.14291570
1        1.24165330     -5.42327727      2.57646099
6        0.91001233     -3.66982179      1.40096710
1       -0.13753350     -3.87896521      1.24462713
6       -2.09521041     -0.71442134     -4.06083443
1       -1.92869170     -1.51685905     -3.34777102
1       -1.96922835     -1.09466087     -5.07804763
6       -3.41546107      0.01623238     -3.88483096
1       -3.61792215      0.14245650     -2.82062143
1       -4.24891932     -0.51426063     -4.34139550
6       -3.13223709      1.37633234     -4.54839743
1       -3.74564859      2.17423666     -4.13806452
1       -3.31056886      1.31593797     -5.62337546
6       -1.64398808      1.62422382     -4.25594301
1       -1.08720579      1.94728012     -5.13605123
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6        1.76964483      3.70043881     -3.90746115
1        2.17252959      4.70571953     -4.01819312
1        0.70599637      3.77501289     -3.67801809
6        2.46269526      2.90762245     -2.80854843
1        3.54785708      3.03931956     -2.82689623
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6        1.29407257     -2.37755871     -4.40760992
1        1.52537077     -1.88212972     -5.35332269
1        0.21695670     -2.48242838     -4.30006619
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1        2.17644572     -4.21374799     -5.20105235
1        1.51212084     -4.35569310     -3.56781877
6        3.38235241     -3.25830475     -3.62503023
1        3.87841299     -4.06664957     -3.09145118
1        4.05913999     -2.88262411     -4.39459207
6        2.95511649     -2.13496601     -2.68405890
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1        3.69940456     -1.34973898     -2.56445569
63      -0.44773493      0.14542728      1.80771655
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7        0.71910751      1.91665124     -0.05466055
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| 1 | 4.52621602 | 3.36044489 | 1.91642402 |
| 6 | 2.75281514 | 2.66696535 | 0.95733808 |
| 1 | 3.27240255 | 1.98522686 | 0.29481934 |
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| 1 | 1.99043148 | 1.35098899 | 5.14032888 |
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| 1 | 4.27012245 | 0.77058875 | 4.40367675 |
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128
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7        0.76085916      -1.56100614       0.07710899
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6        3.05736288      -4.21979470       2.39891493
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1       -3.33494545       1.28778188      -5.69470860
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1        1.53469610      -4.32764925      -3.60790119
6        3.37255534      -3.17340459      -3.67304165
1        3.91980843      -3.97201918      -3.15467391
1        4.03369991      -2.75009698      -4.44594443
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1        3.62928119      -1.28117936      -2.56266352
63      -0.34540761       0.14957465       1.83101416
8        1.14549670      -0.08688578       3.98153001
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| 6 | -3.03615975 | 4.47612283 | -2.33663368 |
| 1 | -3.64710437 | 5.15267593 | -2.93704975 |
| 6 | -1.67250674 | 4.71029426 | -2.15423596 |
| 1 | -1.20862437 | 5.58724592 | -2.61627995 |
| 6 | -0.88077278 | 3.85976436 | -1.38504357 |
| 1 | 0.17522173 | 4.08061466 | -1.22898596 |
| 6 | 2.11559928 | 0.94067995 | 4.19119991 |
| 1 | 1.92752056 | 1.75356482 | 3.47657244 |
| 1 | 2.01730198 | 1.34390323 | 5.21613543 |
| 6 | 3.44145574 | 0.23179453 | 3.99096787 |
| 1 | 3.62137235 | 0.09488266 | 2.91306694 |
| 1 | 4.28954078 | 0.78398807 | 4.41768253 |
| 6 | 3.17412202 | -1.11181823 | 4.67393550 |
| 1 | 3.79183486 | -1.92872036 | 4.28058640 |
| 1 | 3.35614857 | -1.03145375 | 5.75698985 |
| 6 | 1.68677997 | -1.35448077 | 4.38925484 |
| 1 | 1.13710246 | -1.71056257 | 5.27583916 |
| 1 | 1.53461668 | -2.07206122 | 3.56933266 |
| 6 | -2.04427649 | -1.12447776 | 4.67036209 |
| 1 | -1.16583994 | -0.52200850 | 4.94399737 |
| 1 | -2.94700140 | -0.58170909 | 4.99697930 |
| 6 | -1.99292444 | -2.55915258 | 5.23163437 |
| 1 | -1.19371347 | -2.68490825 | 5.97527877 |
| 1 | -2.94280920 | -2.81473433 | 5.72458684 |
| 6 | -1.78123039 | -3.42731106 | 3.98412884 |
| 1 | -2.22630993 | -4.42784751 | 4.07230012 |
| 1 | -0.71009597 | -3.54617390 | 3.75910567 |
| 6 | -2.42686536 | -2.58153905 | 2.89965567 |
| 1 | -3.52901402 | -2.67453827 | 2.90999490 |
| 1 | -2.05638747 | -2.76540147 | 1.88288142 |
| 6 | -1.25768537 | 2.59165058 | 4.47525768 |
| 1 | -1.47109306 | 2.07325807 | 5.42751308 |
| 1 | -0.17104717 | 2.72948906 | 4.38142613 |
| 6 | -2.03430770 | 3.89752972 | 4.35534961 |
| 1 | -2.15774969 | 4.40651274 | 5.32102611 |
| 1 | -1.51349298 | 4.58397737 | 3.67018244 |
| 6 | -3.35135221 | 3.42973271 | 3.73532290 |
| 1 | -3.89860531 | 4.22834730 | 3.21695516 |
| 1 | -4.01249678 | 3.00642510 | 4.50822568 |
| 6 | -2.87502012 | 2.34365607 | 2.77974148 |
| 1 | -2.59347563 | 2.75224140 | 1.79522524 |
| 1 | -3.60807806 | 1.53750748 | 2.62494477 |

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128
Eu_thf_3_2_N2Ph2_2_AV11__Ci__wb97xd_GD2_Def2TZV_MWB53
63       0.46375453       0.11054120      -1.74516349
8       -1.09634016       0.33023220      -3.81532815
8        2.13909787       1.51860747      -3.14002250
8        1.76701995      -1.52836880      -3.31869445
7       -0.68842805      -1.65907512       0.11474169
7        0.78181468      -1.57792884       0.08244175
6       -1.30357782      -2.47760289      -0.79269070
6       -0.64252503      -3.37739615      -1.66883728
1        0.43098418      -3.47344690      -1.59104378
6       -1.36266770      -4.14520360      -2.57780741
1       -0.82968250      -4.83529846      -3.22281378
6       -2.74965183      -4.05875524      -2.66889842
1       -3.29882894      -4.66639598      -3.37431440
6       -3.41842485      -3.18138248      -1.80483601
1       -4.49786678      -3.10033503      -1.85353911
6       -2.72316625      -2.40832410      -0.89558768
1       -3.24089516      -1.71987516      -0.23855933
6        1.47640006      -2.51045796       0.80807494
6        2.87041034      -2.29818275       1.00100317
1        3.30820502      -1.40907371       0.56233009
6        3.63884144      -3.18093670       1.73633958
1        4.69797360      -2.98569198       1.86001136
6        3.06756421      -4.31218105       2.33208769
1        3.67247959      -5.00075121       2.90551993
6        1.70544985      -4.53943914       2.14744381
1        1.24631375      -5.41989675       2.58244886
6        0.91688884      -3.66830505       1.40361022
1       -0.13072332      -3.87704752       1.24738559
6       -2.10266563      -0.70692510      -4.06899764
1       -1.94484568      -1.51056563      -3.35542324
1       -1.97393725      -1.08748018      -5.08573659
6       -3.41976977       0.03096249      -3.89895503
1       -3.62693842       0.15770131      -2.83572444
1       -4.25390509      -0.49433091      -4.36030719
6       -3.12563038       1.38992732      -4.55993859
1       -3.73654672       2.19094419      -4.15193614
1       -3.29884765       1.33130847      -5.63584186
6       -1.63752265       1.62922979      -4.25972153
1       -1.07447507       1.95043133      -5.13650335
1       -1.48837223       2.33854836      -3.44870566
6        2.10410623       1.38739125      -4.59962946
1        1.23945195       0.77183403      -4.83958260
1        3.00772886       0.87194282      -4.92502035
6        2.00383124       2.82309836      -5.15585539
1        1.19760575       2.92065504      -5.88133750
1        2.93398201       3.10843058      -5.64860789
6        1.76720622       3.69815149      -3.90730283
1        2.16926189       4.70371146      -4.01855606
1        0.70322670       3.77188385      -3.67907812
6        2.45963127       2.90707339      -2.80669038
1        3.54480276       3.03882408      -2.82466240
1        2.07649240       3.07753347      -1.80476981
6        1.28472208      -2.37966299      -4.40530703
1        1.50807520      -1.88438127      -5.35301739
1        0.20871576      -2.48899559      -4.29095033
6        2.04474485      -3.69600806      -4.25251465
1        2.17110727      -4.21225731      -5.20265492
1        1.51414007      -4.35704403      -3.56680276
6        3.37993290      -3.25265302      -3.63149092
1        3.88074233      -4.05904727      -3.09939201
1        4.05250937      -2.87512984      -4.40384648
6        2.95266641      -2.13011299      -2.68940238
1        2.65927674      -2.50381113      -1.70813358
1        3.69505773      -1.34265986      -2.57261801
63      -0.44255141       0.14578692       1.80744474
8        1.11754328      -0.07390407       3.87760940
8       -2.11789475      -1.26227935       3.20230375
8       -1.74581683       1.78469692       3.38097570
7        0.70963117       1.91540325      -0.05246044
```

| | | | |
|---|---|---|---|
| 7 | -0.76061156 | 1.83425696 | -0.02016050 |
| 6 | 1.32478095 | 2.73393101 | 0.85497195 |
| 6 | 0.66372816 | 3.63372427 | 1.73111853 |
| 1 | -0.40978105 | 3.72977502 | 1.65332503 |
| 6 | 1.38387083 | 4.40153173 | 2.64008866 |
| 1 | 0.85088563 | 5.09162658 | 3.28509503 |
| 6 | 2.77085495 | 4.31508337 | 2.73117967 |
| 1 | 3.32003207 | 4.92272410 | 3.43659565 |
| 6 | 3.43962798 | 3.43771061 | 1.86711726 |
| 1 | 4.51906990 | 3.35666316 | 1.91582036 |
| 6 | 2.74436938 | 2.66465222 | 0.95786893 |
| 1 | 3.26209829 | 1.97620328 | 0.30084058 |
| 6 | -1.45519693 | 2.76678608 | -0.74579369 |
| 6 | -2.84920722 | 2.55451087 | -0.93872192 |
| 1 | -3.28700190 | 1.66540184 | -0.50004884 |
| 6 | -3.61763832 | 3.43726482 | -1.67405833 |
| 1 | -4.67677048 | 3.24202011 | -1.79773011 |
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| 6 | -1.68424672 | 4.79576727 | -2.08516256 |
| 1 | -1.22511063 | 5.67622488 | -2.52016761 |
| 6 | -0.89568572 | 3.92463317 | -1.34132897 |
| 1 | 0.15192644 | 4.13337565 | -1.18510434 |
| 6 | 2.12386876 | 0.96325323 | 4.13127889 |
| 1 | 1.96604880 | 1.76689375 | 3.41770449 |
| 1 | 1.99514037 | 1.34380831 | 5.14801784 |
| 6 | 3.44097290 | 0.22536563 | 3.96123628 |
| 1 | 3.64814154 | 0.09862681 | 2.89800569 |
| 1 | 4.27510822 | 0.75065904 | 4.42258844 |
| 6 | 3.14683351 | -1.13359919 | 4.62221984 |
| 1 | 3.75774984 | -1.93461607 | 4.21421739 |
| 1 | 3.32005077 | -1.07498035 | 5.69812311 |
| 6 | 1.65872577 | -1.37290167 | 4.32200278 |
| 1 | 1.09567820 | -1.69410321 | 5.19878460 |
| 1 | 1.50957535 | -2.08222024 | 3.51098691 |
| 6 | -2.08290311 | -1.13106312 | 4.66191071 |
| 1 | -1.21824883 | -0.51550590 | 4.90186385 |
| 1 | -2.98652574 | -0.61561470 | 4.98730160 |
| 6 | -1.98262811 | -2.56677024 | 5.21813664 |
| 1 | -1.17640262 | -2.66432692 | 5.94361875 |
| 1 | -2.91277888 | -2.85210245 | 5.71088914 |
| 6 | -1.74600310 | -3.44182337 | 3.96958408 |
| 1 | -2.14805876 | -4.44738334 | 4.08083731 |
| 1 | -0.68202357 | -3.51555572 | 3.74135937 |
| 6 | -2.43842815 | -2.65074527 | 2.86897163 |
| 1 | -3.52359963 | -2.78249596 | 2.88694365 |
| 1 | -2.05528928 | -2.82120534 | 1.86705106 |
| 6 | -1.26351895 | 2.63599112 | 4.46758828 |
| 1 | -1.48687207 | 2.14070940 | 5.41529864 |
| 1 | -0.18751263 | 2.74532371 | 4.35323158 |
| 6 | -2.02354173 | 3.95233618 | 4.31479590 |
| 1 | -2.14990414 | 4.46858544 | 5.26493617 |
| 1 | -1.49293694 | 4.61337215 | 3.62908401 |
| 6 | -3.35872977 | 3.50898114 | 3.69377217 |
| 1 | -3.85953921 | 4.31537539 | 3.16167326 |
| 1 | -4.03130625 | 3.13145797 | 4.46612773 |
| 6 | -2.93146329 | 2.38644112 | 2.75168363 |
| 1 | -2.63807361 | 2.76013925 | 1.77041483 |
| 1 | -3.67385461 | 1.59898799 | 2.63489926 |

Table S3. Differences from experiment (**Å**) for symmetry-unique Eu-R (R = Eu/O/N/Cp) interatomic distances across theoretical methods. Experimental values are provided at table bottom.

| Method | Eu-Eu | Eu-O1 | Eu-O2 | Eu-O3 | Eu-N1 | Eu-N2 | Eu-N3 | Eu-N4 | Eu-C1 | Eu-C2 |
|---|---|---|---|---|---|---|---|---|---|---|
| B3LYP/Def2-SVP | 0.037 | 0.098 | 0.091 | 0.086 | 0.100 | 0.074 | 0.053 | 0.048 | 0.103 | 0.121 |
| B3LYP/Def2-TZV | 0.046 | 0.083 | 0.055 | 0.065 | 0.148 | 0.073 | 0.055 | 0.095 | 0.202 | 0.201 |
| B3LYP-GD3(BJ)/Def2-SVP | 0.024 | 0.032 | 0.009 | -0.007 | 0.115 | 0.053 | 0.023 | 0.029 | 0.065 | 0.094 |
| B3LYP-GD3(BJ)/Def2-TZV | 0.016 | 0.013 | -0.017 | -0.027 | 0.144 | 0.049 | 0.023 | 0.057 | 0.133 | 0.159 |
| CAM-B3LYP/Def2-SVP | 0.000 | 0.070 | 0.047 | 0.041 | 0.072 | 0.065 | 0.043 | 0.031 | 0.052 | 0.087 |
| CAM-B3LYP/Def2-TZV | 0.000 | 0.049 | 0.010 | 0.017 | 0.116 | 0.061 | 0.044 | 0.071 | 0.155 | 0.167 |
| CAM-B3LYP-GD3(BJ)/Def2-SVP | -0.015 | 0.031 | 0.003 | -0.008 | 0.078 | 0.053 | 0.023 | 0.015 | 0.029 | 0.072 |
| CAM-B3LYP-GD3(BJ)/Def2-TZV | -0.022 | 0.011 | -0.027 | -0.032 | 0.115 | 0.047 | 0.022 | 0.046 | 0.117 | 0.148 |
| LC-ωHPBE/Def2-SVP | -0.006 | 0.075 | 0.058 | 0.059 | 0.051 | 0.056 | 0.038 | 0.000 | 0.036 | 0.021 |
| LC-ωHPBE/Def2-TZV | -0.011 | 0.045 | 0.015 | -0.009 | 0.028 | 0.046 | 0.028 | -0.003 | 0.034 | -0.050 |
| LC-ωHPBE-GD3(BJ)/Def2-SVP | -0.007 | 0.052 | 0.018 | -0.014 | 0.033 | 0.046 | 0.030 | 0.001 | 0.037 | -0.041 |
| LC-ωHPBE-GD3(BJ)/Def2-TZV | -0.036 | 0.024 | -0.003 | -0.030 | 0.049 | 0.037 | 0.022 | 0.028 | 0.110 | 0.043 |
| ωB97XD/Def2-SVP | 0.047 | 0.036 | 0.009 | -0.018 | 0.092 | 0.062 | 0.027 | 0.022 | -0.014 | 0.053 |
| ωB97XD/Def2-TZV | 0.047 | 0.009 | -0.021 | -0.039 | 0.151 | 0.051 | 0.018 | 0.049 | 0.091 | 0.141 |
| ωB97XD-GD2/Def2-SVP | 0.048 | 0.036 | 0.008 | -0.017 | 0.097 | 0.062 | 0.027 | 0.012 | -0.009 | 0.045 |
| ωB97XD-GD2/Def2-TZV | 0.044 | 0.010 | -0.022 | -0.039 | 0.143 | 0.052 | 0.018 | 0.053 | 0.087 | 0.143 |
| Experiment | 3.622 | 2.592 | 2.617 | 2.658 | 2.671 | 2.456 | 2.469 | 2.676 | 3.189 | 3.283 |

Table S4. RMSD, NPA natural charges, N=N stretching modes, gas-phase frequencies ($cm^{-1}$) for cis-azobenzene, and average time-per-SCF cycle (SCF, min:sec) on a 16-core 3.3 GHz computer.

| Method | RMSD | $NPA_{Eu}$ | $NPA_{N1}$ | $NPA_{N2}$ | Ng | Nu | N-cis | % vs. Exp. | N NPA | SCF |
|---|---|---|---|---|---|---|---|---|---|---|
| B3LYP/Def2-SVP | 0.284 | 1.572 | -0.676 | -0.690 | 1003 | 1004 | 1679 | 11.1 | -0.142 | 10:36 |
| B3LYP/Def2-TZV | 0.358 | 1.238 | -0.615 | -0.621 | 1009 | 1010 | 1472 | -2.6 | -0.106 | 25:06 |
| B3LYP-GD3(BJ)/Def2-SVP | 0.305 | 1.520 | -0.664 | -0.680 | 1012 | 1013 | 1679 | 11.1 | -0.143 | 11:22 |
| B3LYP-GD3(BJ)/Def2-TZV | 0.309 | 1.211 | -0.597 | -0.594 | 1016 | 1016 | 1471 | -2.6 | -0.106 | 25:57 |
| CAM-B3L/YP/Def2-SVP | 0.288 | 1.498 | -0.699 | -0.710 | 1032 | 1033 | 1751 | 15.9 | -0.139 | 14:47 |
| CAM-B3LYP/Def2-TZV | 0.312 | 1.247 | -0.616 | -0.626 | 1029 | 1030 | 1566 | 3.6 | -0.104 | 37:24 |
| CAM-B3LYP-GD3(BJ)/Def2-SVP | 0.285 | 1.476 | -0.680 | -0.693 | 1036 | 1038 | 1750 | 15.8 | -0.139 | 20:02 |
| CAM-B3LYP-GD3(BJ)/Def2-TZV | 0.296 | 1.236 | -0.604 | -0.616 | 1032 | 1033 | 1564 | 3.5 | -0.104 | 32:32 |
| LC-ωHPBE/Def2-SVP | 0.231 | 1.513 | -0.690 | -0.708 | 1071 | 1073 | 1815 | 20.1 | -0.133 | 22:02 |
| | | | | | 1060 | 1062 | | | | |
| LC-ωHPBE/Def2-TZV | 0.151 | 1.287 | -0.619 | -0.634 | 997 | 1002 | 1642 | 8.6 | -0.097 | 48:41 |
| | | | | | 1042 | 1043 | | | | |
| LC-ωHPBE-GD3(BJ)/Def2-SVP | 0.165 | 1.493 | -0.688 | -0.691 | 1063 | 1064 | 1811 | 19.8 | -0.133 | 18:21 |
| | | | | | 1074 | 1076 | | | | |
| LC-ωHPBE-GD3(BJ)/Def2-TZV | 0.178 | 1.239 | -0.614 | -0.613 | 1002 | 1005 | 1639 | 8.4 | -0.097 | 39:22 |
| | | | | | 1046 | 1047 | | | | |
| ωB97XD/Def2-SVP | 0.319 | 1.494 | -0.679 | -0.692 | 1039 | 1041 | 1740 | 15.2 | -0.140 | 18:39 |
| ωB97XD/Def2-TZV | 0.325 | 1.224 | -0.599 | -0.616 | 1030 | 1030 | 1559 | 3.1 | -0.101 | 39:42 |
| ωB97XD-GD2/Def2-SVP | 0.318 | 1.497 | -0.678 | -0.690 | 1039 | 1041 | 1740 | 15.2 | -0.140 | 16:42 |
| ωB97XD-GD2/Def2-TZV | 0.324 | 1.224 | -0.598 | -0.617 | 1030 | 1030 | 1559 | 3.1 | -0.101 | 36:17 |