

Supporting Information:

Modulating Electronic Properties of Dinitrosoarene Polymers

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Geometry optimization. We tested the Perdew, Burke and Ernzerhof (PBE¹) functional and PBEsol², the meta-GGA TPSS³ functional, the vdW-DF2⁴ and vdW-DF2-B86R⁵ flavors of the van der Waals density functional, and the SCAN-rVV10⁶ method. For PBE variants and TPSS, long-range interactions were modeled using Grimme's D3BJ scheme,⁷ revised D3BJ scheme⁸ the dDsC method^{9,10}, many-body dispersion energy scheme (MBD)^{11,12}, and the Tkatchenko-Scheffler (TS) method.¹³ The comparison between the obtained results is shown in Figure S1.

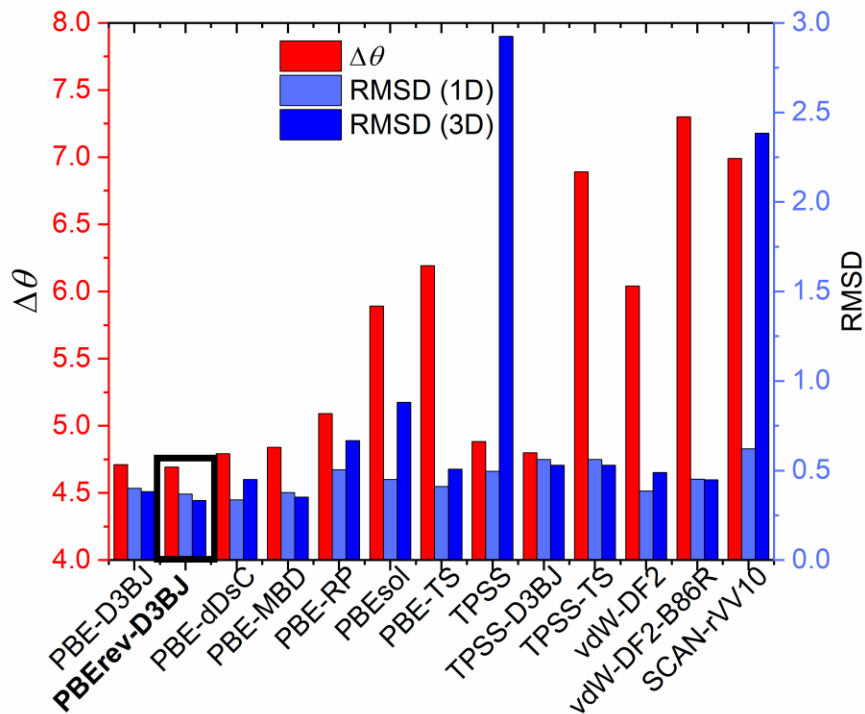


Figure S1. Torsional angle (red) deviations and RMSD (blue) values between the experimental and calculated structures of **1c**, obtained using different functionals and dispersion corrections. Hydrogen atoms were not considered during the RMSD calculation.

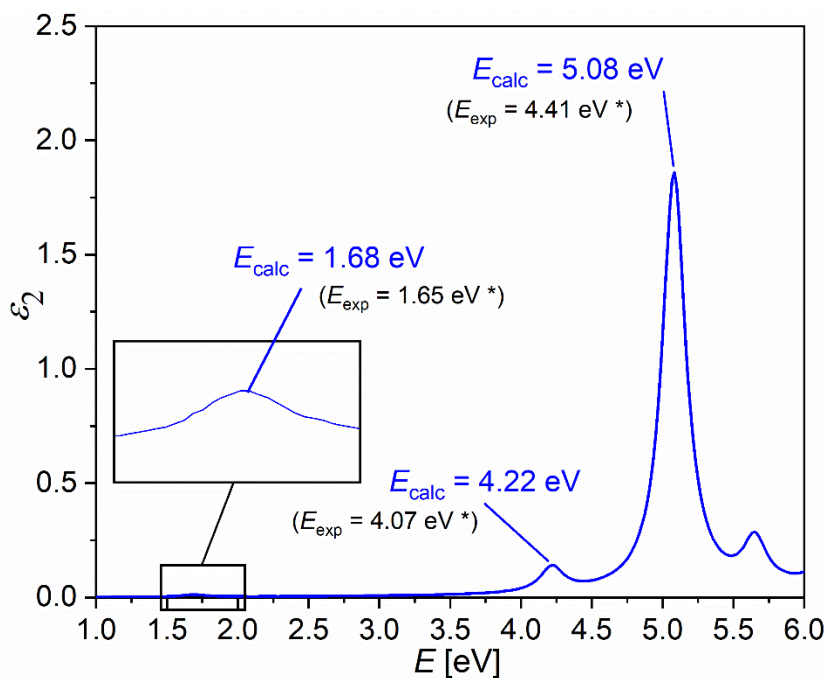


Figure S2. Calculated optical spectrum of monomer of 1,4-dinitrosobenzene using the HSE functional. Calculated peaks are compared to *J.Phys.Chem.* **1996**, *10*, 11883-11892.

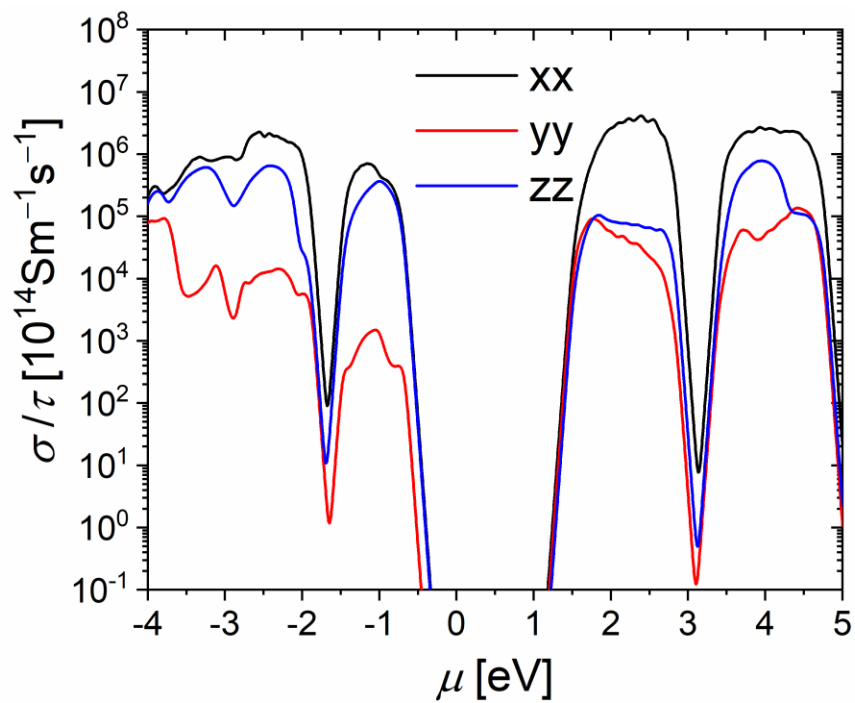


Figure S3. Conductivity vs chemical potential of **C1** in x (black), y (red), and z (blue) direction of the unit cell at 300 K, calculated using the HSE functional.

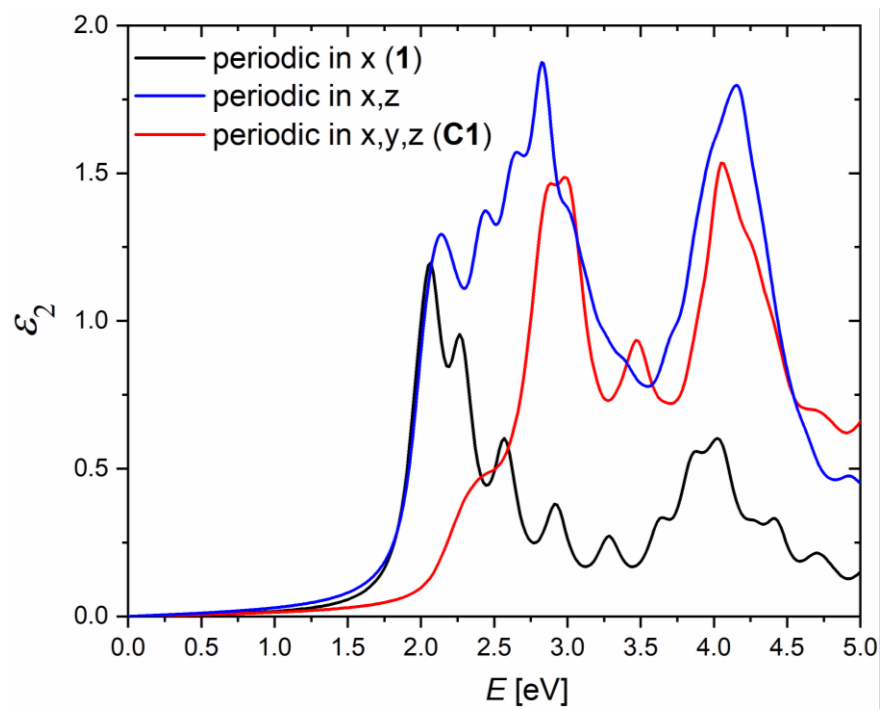


Figure S4. Comparison of optical spectra of **1** (black), **C1** (red) and **1** stacked in z direction of the unit cell (blue).

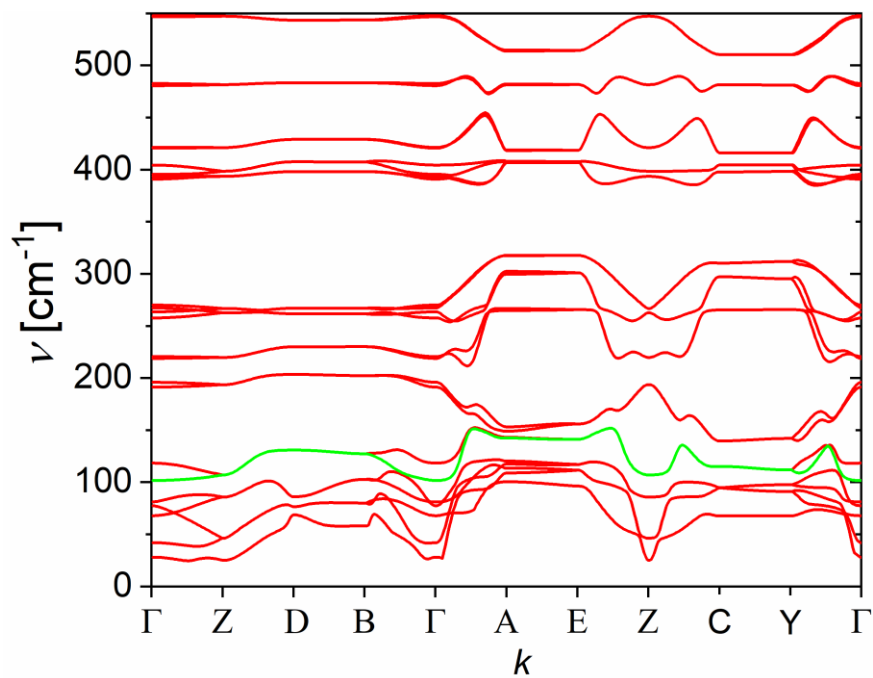


Figure S5. Full phonon band structure of **C1**.

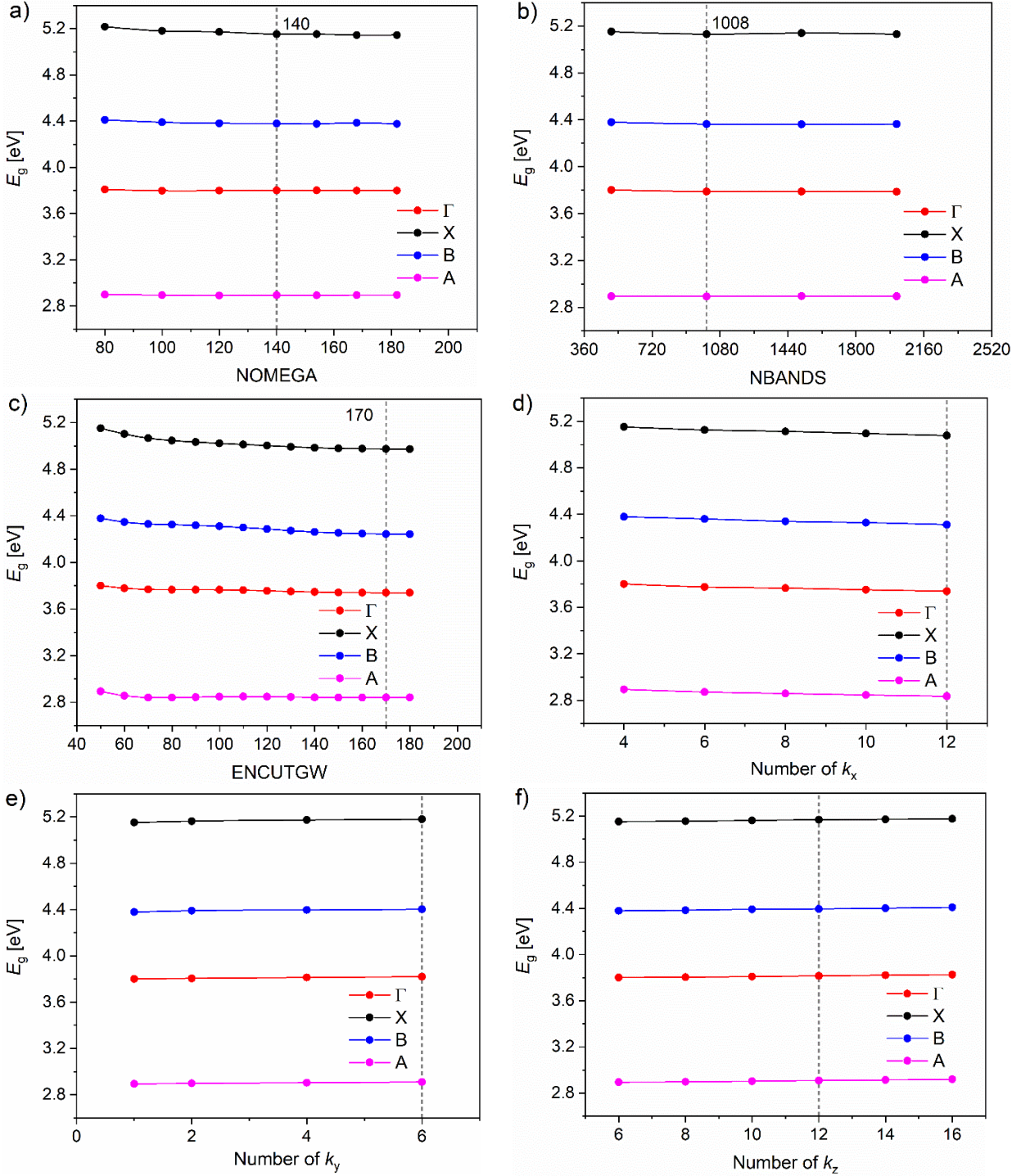


Figure S6. GW convergence with respect to the number of sampled frequencies (NOMEGA, a), number of bands (NBANDS, b), plane wave kinetic energy cutoff (ENCUTGW, c), and k-mesh density in the x (d), y (e), and z (f) directions.

Table S1. Obtained zero-gap renormalization (ZGR, in eV) values with different supercells.

| supercell | ZGR | supercell | ZGR |
|-----------|--------------|-----------|--------------|
| 222 | -0.44 | 222 | 0.02 |
| 322 | -0.46 | 223 | 0.41 |
| 422 | -0.22 | 224 | -0.14 |
| 522 | -0.26 | 225 | -0.24 |
| 622 | -0.27 | 226 | -0.27 |

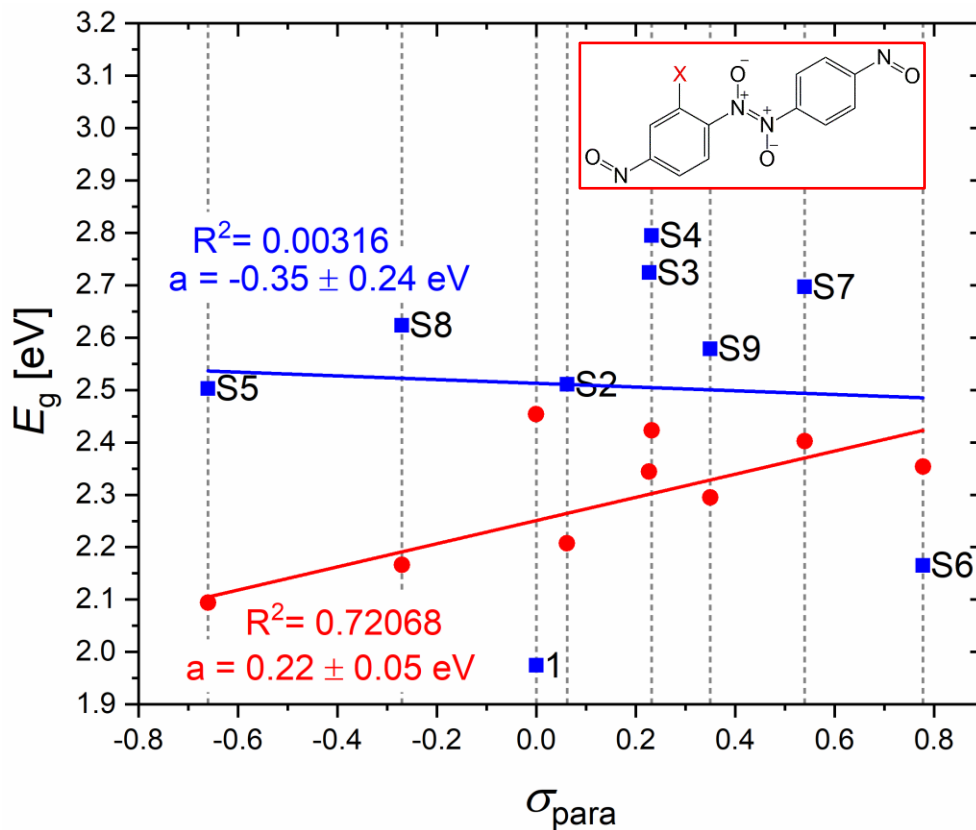


Figure S7. Hammett-type plots for dimers (red, dimer structure shown in insert with red borders) and polymers (blue), with corresponding correlation parameters.

Optimized Geometries

POLYMERS

1

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1.0000000000000000

| | | |
|---------------------|---------------------|---------------------|
| 6.4803362089090477 | -0.0143219035236095 | -0.0136943423225076 |
| -0.0340745981802522 | 15.1963758046032318 | 0.1238532346934939 |
| -0.4897431126667838 | 0.1007394958621814 | 11.6646310666145379 |

| | | | |
|---|---|---|---|
| O | N | C | H |
| 2 | 2 | 6 | 4 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.5266853216986433 | 0.5964007030313354 | 0.5308407670777484 |
| 0.4817547983020631 | 0.3827684931597517 | 0.4351512560098882 |
| 0.5765260686329086 | 0.5202955096742627 | 0.4977789713942400 |
| 0.4321003478241465 | 0.4589301363235307 | 0.4679462897153925 |
| 0.9174146505829341 | 0.5720483141094448 | 0.4591677180228046 |
| 0.7925466142958228 | 0.5001532046630999 | 0.4874583935836654 |
| 0.8790877591577555 | 0.4172211108746993 | 0.5116840642246316 |
| 0.0913659796576241 | 0.4071397178575040 | 0.5064843607953691 |
| 0.2161686682552570 | 0.4790561084728040 | 0.4783024928581199 |
| 0.1296268190936942 | 0.5619580079733666 | 0.4539481471845548 |
| 0.8458055288074533 | 0.6358073942120654 | 0.4423104277942187 |
| 0.7828788251815197 | 0.3615214971824443 | 0.5339943667474358 |
| 0.1629957974738829 | 0.3433594292111195 | 0.5231626066724573 |
| 0.2259428907655661 | 0.6176003708546034 | 0.4315200272087125 |

C1

Comment

1.0000000000000000

| | | |
|---------------------|---------------------|---------------------|
| 6.4082532264819854 | 0.0000000000000000 | -0.0204061826993043 |
| 0.0000000000000000 | 11.3385703635430275 | 0.0000000000000000 |
| -0.1549602393918430 | 0.0000000000000000 | 3.6202320954588298 |

| | | | |
|---|---|----|---|
| O | N | C | H |
| 4 | 4 | 12 | 8 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.5181479461501581 | 0.6276623354804869 | 0.2559636591053334 |
| 0.4818520538498490 | 0.3723376645195131 | 0.7440363708946620 |
| 0.9818520538498419 | 0.1276623354804869 | 0.2440363408946666 |
| 0.0181479461501510 | 0.8723376645195131 | 0.7559636291053380 |
| 0.5704425163438316 | 0.5370898694991340 | 0.0759364123198267 |
| 0.4295574836561684 | 0.4629101305008660 | 0.9240636106801787 |
| 0.9295574836561684 | 0.0370898694991340 | 0.4240635806801762 |
| 0.0704425163438316 | 0.9629101305008660 | 0.5759363893198213 |
| 0.9079545626362844 | 0.6088130942160248 | 0.9091486995144891 |
| 0.0920454373637156 | 0.3911869057839752 | 0.0908513004855109 |
| 0.5920454373637156 | 0.1088130942160248 | 0.5908513004855109 |
| 0.4079545626362844 | 0.8911869057839752 | 0.4091486995144891 |
| 0.7890411453536359 | 0.5140343668498417 | 0.0256759716423716 |
| 0.2109588546463641 | 0.4859656331501583 | 0.9743240133576307 |
| 0.7109588546463641 | 0.0140343668498417 | 0.4743240133576307 |
| 0.2890411453536359 | 0.9859656331501583 | 0.5256759866423693 |
| 0.8780892359122490 | 0.4051910204846152 | 0.1178970713640624 |

| | | |
|--------------------|--------------------|--------------------|
| 0.1219107640877510 | 0.5948089495153894 | 0.8821029056359393 |
| 0.6219107640877510 | 0.9051910504846106 | 0.3821029356359347 |
| 0.3780892359122490 | 0.0948089795153848 | 0.6178970943640607 |
| 0.8339778120751475 | 0.6923650423789240 | 0.8361578867443740 |
| 0.1660221879248525 | 0.3076349576210760 | 0.1638420992556249 |
| 0.6660221879248525 | 0.1923650423789240 | 0.6638421132556260 |
| 0.3339778120751475 | 0.8076349576210760 | 0.3361578867443740 |
| 0.7839771785715897 | 0.3327608416113392 | 0.2134695953351127 |
| 0.2160228214284103 | 0.6672391883886633 | 0.7865304196648850 |
| 0.7160228214284103 | 0.8327608116113367 | 0.2865304196648850 |
| 0.2839771785715897 | 0.1672391583886608 | 0.7134695803351150 |

1@Au

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|--------------------|---------------------|---------------------|
| 1.0000000000000000 | | |
| 8.7390003204000006 | 0.0000000000000000 | 0.0000000000000000 |
| 1.4564987788999999 | 17.6591378572000011 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 30.0000000000000000 |

| | | | | |
|-----|---|---|----|----|
| Au | O | N | C | H |
| 105 | 6 | 6 | 18 | 12 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.7653800249999989 | 0.1022199989999990 | 0.1990400549999976 |
| 0.9077200290000036 | 0.2452699990000013 | 0.1991100309999965 |
| 0.0500200019999966 | 0.3882400099999970 | 0.1991399529999995 |
| 0.1926899999999989 | 0.5309100150000035 | 0.1994800570000024 |
| 0.3360300060000014 | 0.6736500259999971 | 0.1996300220000009 |
| 0.4794700149999969 | 0.8162900210000004 | 0.1994899509999968 |
| 0.6226500269999988 | 0.9591900109999969 | 0.1993800400000012 |
| 0.4321300089999980 | 0.1023100020000030 | 0.1990300419999969 |
| 0.5743499989999989 | 0.2452899959999968 | 0.1989400390000000 |
| 0.7166399959999978 | 0.3883000020000011 | 0.1990000010000017 |
| 0.8593699930000014 | 0.5309600229999987 | 0.1993299720000010 |
| 0.0025100000000009 | 0.6735699769999997 | 0.1994099619999972 |
| 0.1461900030000010 | 0.8163400290000027 | 0.1994999650000011 |
| 0.2892000080000017 | 0.9592400189999992 | 0.1991900209999997 |
| 0.0985800030000021 | 0.1022099999999995 | 0.1991200450000008 |
| 0.2411800029999966 | 0.2453700009999977 | 0.1992199419999992 |
| 0.3832499979999966 | 0.3882699910000014 | 0.1991499660000002 |
| 0.5260000230000017 | 0.5309600229999987 | 0.1994999650000011 |
| 0.6691100000000034 | 0.6736199859999985 | 0.1995199919999990 |
| 0.8126999739999974 | 0.8162699940000024 | 0.1995699410000000 |
| 0.9559199810000010 | 0.9592800140000008 | 0.1993999479999999 |
| 0.6057500240000024 | 0.0528800000000018 | 0.2794600129999978 |
| 0.7486000059999967 | 0.1958999929999976 | 0.2793099880000014 |
| 0.8912100200000026 | 0.3390200139999990 | 0.2794399859999999 |
| 0.0335000010000002 | 0.4818499980000013 | 0.2798599899999985 |
| 0.1763599960000022 | 0.6245099900000000 | 0.2800599930000018 |
| 0.3191800119999968 | 0.7671499850000032 | 0.2801699939999978 |
| 0.4624600109999975 | 0.9098899959999969 | 0.2797099949999975 |
| 0.2724600140000035 | 0.0529799979999979 | 0.2793900070000035 |
| 0.4153299930000003 | 0.1959899960000016 | 0.2793000039999995 |
| 0.5578699710000024 | 0.3390299980000009 | 0.2793399990000012 |
| 0.7002500299999994 | 0.4818499980000013 | 0.2797200079999982 |
| 0.8430299759999969 | 0.6244599819999976 | 0.2799200119999981 |

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|--------------------|--------------------|--------------------|
| 0.9860500099999996 | 0.7671200039999988 | 0.2799699899999979 |
| 0.1292299930000027 | 0.9099799990000008 | 0.2796899969999984 |
| 0.9389600160000029 | 0.0530199999999965 | 0.2795700129999972 |
| 0.0819299970000031 | 0.1960600020000030 | 0.2794800100000003 |
| 0.2244600060000010 | 0.3392300009999971 | 0.2796500030000004 |
| 0.3666599989999995 | 0.4820699989999966 | 0.2800399959999993 |
| 0.5094900129999971 | 0.6245499850000016 | 0.2802500129999999 |
| 0.6523399949999984 | 0.7671399709999989 | 0.2801800069999985 |
| 0.7957299950000021 | 0.9098399880000017 | 0.2799099980000008 |
| 0.7779200080000024 | 0.0020200000000017 | 0.3580600020000020 |
| 0.9210500120000020 | 0.1450600029999976 | 0.3578499850000014 |
| 0.0637900010000010 | 0.2882399860000007 | 0.3579599859999973 |
| 0.2065899970000018 | 0.4312900010000007 | 0.3583700060000012 |
| 0.3488399980000025 | 0.5742499830000014 | 0.3590199949999970 |
| 0.4917300050000009 | 0.7165600060000017 | 0.3589600030000000 |
| 0.6343100070000034 | 0.8591399789999983 | 0.3586499990000007 |
| 0.4447500109999964 | 0.0020000000000024 | 0.3578499850000014 |
| 0.5877900119999993 | 0.1450199929999982 | 0.3576000030000017 |
| 0.7307599780000018 | 0.2880100010000035 | 0.3575800059999992 |
| 0.8734599949999975 | 0.4309799970000014 | 0.3580699859999967 |
| 0.0161799990000020 | 0.5738899709999998 | 0.3585000039999997 |
| 0.1587599960000006 | 0.7163900139999981 | 0.3587400019999976 |
| 0.3016200069999968 | 0.8592500090000001 | 0.3583999869999985 |
| 0.1114299970000019 | 0.0020499999999970 | 0.3579599859999973 |
| 0.2545099849999986 | 0.1449799979999966 | 0.3577300010000002 |
| 0.3973900080000021 | 0.2880699930000006 | 0.3577199879999995 |
| 0.5400300029999983 | 0.4310300049999967 | 0.3580200079999969 |
| 0.6829500199999998 | 0.5737500190000020 | 0.3585200010000023 |
| 0.8255199789999992 | 0.7163199780000014 | 0.3585300149999995 |
| 0.9687100049999984 | 0.8590400220000021 | 0.3584299979999983 |
| 0.7604100109999976 | 0.0942599999999985 | 0.4363200069999991 |
| 0.9024099709999973 | 0.2369700069999965 | 0.4362800119999974 |
| 0.0449200010000013 | 0.3801000119999998 | 0.4368900059999987 |
| 0.1871699989999982 | 0.5228800180000022 | 0.4374400080000029 |
| 0.3313199879999971 | 0.6661800150000019 | 0.4382799859999977 |
| 0.4738300140000007 | 0.8083999750000004 | 0.4377099869999981 |
| 0.6180700059999964 | 0.9513400200000035 | 0.4368900059999987 |
| 0.4280500110000034 | 0.0939199999999971 | 0.4359099859999986 |
| 0.5698300000000032 | 0.2369499950000034 | 0.4357500079999994 |
| 0.7119500040000020 | 0.3796600100000020 | 0.4360300000000024 |
| 0.8557800049999997 | 0.5223199730000019 | 0.4367600080000003 |
| 0.9982799889999967 | 0.6655099990000011 | 0.4371399879999984 |
| 0.1427499950000026 | 0.8080999849999984 | 0.4371399879999984 |
| 0.2852399949999977 | 0.9514700169999983 | 0.4364300069999985 |
| 0.0934899969999989 | 0.0945300010000025 | 0.4361400009999983 |
| 0.2351800049999966 | 0.2373400029999999 | 0.4358800050000013 |
| 0.3776099979999969 | 0.3802399930000036 | 0.4362500009999977 |
| 0.5204899909999980 | 0.5232200029999987 | 0.4365600049999969 |
| 0.6642600300000012 | 0.6655899880000007 | 0.4370799960000014 |
| 0.8075199720000015 | 0.8086799980000023 | 0.4366999860000007 |
| 0.9505299930000035 | 0.9514499900000004 | 0.4363999959999987 |
| 0.6022099850000018 | 0.0450600010000031 | 0.5172700290000023 |
| 0.7418699859999975 | 0.1875000000000000 | 0.5170000199999976 |
| 0.8829900030000033 | 0.3297599850000026 | 0.5168700219999991 |

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|--------------------|--------------------|--------------------|
| 0.0255500000000026 | 0.4724200069999966 | 0.5187000040000029 |
| 0.1702200029999972 | 0.6160600190000025 | 0.5180100199999984 |
| 0.3152300120000007 | 0.7595999839999976 | 0.5195999740000019 |
| 0.4596599939999990 | 0.9027500150000023 | 0.5175499919999993 |
| 0.2675499919999993 | 0.0461799990000031 | 0.5157399770000026 |
| 0.4079900090000024 | 0.1880999950000017 | 0.5149800180000028 |
| 0.5483899709999989 | 0.3303500119999967 | 0.5155400040000018 |
| 0.6911600230000019 | 0.4728800059999969 | 0.5155000090000001 |
| 0.8360000249999970 | 0.6154000160000024 | 0.5164800290000002 |
| 0.9800000190000020 | 0.7598000170000034 | 0.5161899920000010 |
| 0.1249099970000032 | 0.9031299950000005 | 0.5156800150000009 |
| 0.9341700080000024 | 0.0453100020000008 | 0.5168200139999968 |
| 0.0747099969999994 | 0.1881899979999986 | 0.5171700120000011 |
| 0.2163099939999995 | 0.3301500079999968 | 0.5171899799999977 |
| 0.3583999869999985 | 0.4734399909999993 | 0.5172899960000024 |
| 0.5037800070000031 | 0.6155800220000032 | 0.5184599760000026 |
| 0.6479600070000018 | 0.7590900060000010 | 0.5174199940000008 |
| 0.7921800020000020 | 0.9023100140000011 | 0.5180600289999973 |
| 0.2938899990000010 | 0.2255100010000035 | 0.6297399999999982 |
| 0.6278899910000035 | 0.1111100019999967 | 0.6148200040000020 |
| 0.6259099840000033 | 0.5593399999999988 | 0.6289899949999977 |
| 0.9602000120000014 | 0.4460699859999977 | 0.6129099730000007 |
| 0.9618899820000024 | 0.8916500209999967 | 0.6337400079999966 |
| 0.2899500130000021 | 0.7792900199999977 | 0.6074200270000034 |
| 0.4365200100000024 | 0.2067199950000003 | 0.6255800129999969 |
| 0.4857999979999974 | 0.1297899930000028 | 0.6217700239999999 |
| 0.7685099839999978 | 0.5406500100000002 | 0.6248700020000015 |
| 0.8181300159999978 | 0.4641000029999987 | 0.6206700210000022 |
| 0.1023999969999991 | 0.8734899760000019 | 0.6255800129999969 |
| 0.1503300070000009 | 0.7970799799999995 | 0.6194199919999974 |
| 0.4695700110000018 | 0.3425799910000009 | 0.6233599780000034 |
| 0.5429900290000020 | 0.2681399880000015 | 0.6243199709999985 |
| 0.7056900259999992 | 0.2625299990000016 | 0.6245200039999972 |
| 0.4531100089999995 | 0.9938899870000029 | 0.6241700050000034 |
| 0.3802100119999992 | 0.0685200019999996 | 0.6236699820000027 |
| 0.2173800019999987 | 0.0744400020000029 | 0.6227099899999970 |
| 0.8016999959999964 | 0.6765499710000000 | 0.6235299709999964 |
| 0.8748400209999971 | 0.6020699740000026 | 0.6231999990000006 |
| 0.0377399999999994 | 0.5961300129999998 | 0.6228200199999989 |
| 0.7871400120000018 | 0.3278799950000035 | 0.6237599849999995 |
| 0.7134900089999974 | 0.4022899870000032 | 0.6232600210000001 |
| 0.5508499740000019 | 0.4078699949999987 | 0.6231399770000010 |
| 0.1353899989999974 | 0.0093600000000009 | 0.6229599710000002 |
| 0.2083999959999971 | 0.9349499940000001 | 0.6235299709999964 |
| 0.3711400030000007 | 0.9288300280000001 | 0.6239799860000019 |
| 0.1194999960000018 | 0.6612300279999985 | 0.6220499869999969 |
| 0.0461600009999970 | 0.7358000279999999 | 0.6223499769999989 |
| 0.8833900090000029 | 0.7416599989999995 | 0.6232900019999974 |
| 0.3443199989999997 | 0.3496699929999991 | 0.6228100060000017 |
| 0.7706999780000032 | 0.2074999960000028 | 0.6251999739999974 |
| 0.5783299799999995 | 0.9864900110000008 | 0.6246100070000011 |
| 0.1530099960000015 | 0.1295900049999972 | 0.6216300130000008 |
| 0.6764600280000010 | 0.6837199929999969 | 0.6238499880000035 |
| 0.1023600030000011 | 0.5410199760000012 | 0.6229000089999985 |

| | | |
|--------------------|--------------------|--------------------|
| 0.9124299879999995 | 0.3207100030000021 | 0.6239699719999976 |
| 0.4858700039999988 | 0.4628700020000025 | 0.6220300199999969 |
| 0.0101099999999974 | 0.0167500000000018 | 0.6224799749999974 |
| 0.4354400040000002 | 0.8735600110000021 | 0.6245700119999995 |
| 0.2447700049999995 | 0.6539300080000032 | 0.6215999719999985 |
| 0.8189200159999999 | 0.7968000170000025 | 0.6232699749999995 |

S2

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| | | |
|---------------------|---------------------|---------------------|
| 1.0000000000000000 | | |
| 6.4188813054613476 | -0.0090701928859537 | -0.0039056118087929 |
| -0.0212430072573395 | 15.0406033687833531 | 0.0822237838203068 |
| -0.4683925741175907 | 0.0661680049572238 | 11.8964076190030994 |

| | | | | | |
|---|---|---|---|---|--|
| O | N | C | H | F | |
| 2 | 2 | 6 | 3 | 1 | |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.5159948607808431 | 0.5851243700238413 | 0.5596285765754274 |
| 0.4860893998758726 | 0.3950792898156905 | 0.3984814472485638 |
| 0.5697601152697942 | 0.5162842124620681 | 0.5067938114434938 |
| 0.4307378344775614 | 0.4607774899379180 | 0.4560130269179226 |
| 0.9097712682428565 | 0.5702986700551733 | 0.4561909619561817 |
| 0.7872409836215013 | 0.4990227656363260 | 0.4912769605849974 |
| 0.8815393456479867 | 0.4175492706792312 | 0.5191987645342593 |
| 0.0936262423891137 | 0.4051925285005069 | 0.5072862879279043 |
| 0.2118316851826734 | 0.4773164253266984 | 0.4717972847013314 |
| 0.1230862593399067 | 0.5601768832962932 | 0.4464764200364755 |
| 0.8340541912454924 | 0.6338092194198168 | 0.4381265160325114 |
| 0.1654789073688860 | 0.3411061965477558 | 0.5265739972678460 |
| 0.2191110742167695 | 0.6156373229372392 | 0.4203509414717530 |
| 0.7682556853407689 | 0.3505586693614546 | 0.5624095963013076 |

S3

Comment

| | | |
|---------------------|---------------------|---------------------|
| 1.0000000000000000 | | |
| 6.4100375850297144 | -0.0130138479256447 | -0.0030387000900931 |
| -0.0305140920808658 | 15.0312594627528355 | 0.1080761476338868 |
| -0.4662239338576516 | 0.0871721511520409 | 11.9204479972085942 |

| | | | | | |
|---|---|---|---|----|--|
| O | N | C | H | Cl | |
| 2 | 2 | 6 | 3 | 1 | |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.5132093798123591 | 0.5737060522891611 | 0.5697404174648426 |
| 0.4821960784531782 | 0.4008857099752063 | 0.3815573443656746 |
| 0.5673327161915367 | 0.5103100831030503 | 0.5077081947823388 |
| 0.4281022758861752 | 0.4609647909287204 | 0.4479262780191888 |
| 0.9046986899688747 | 0.5672937446537958 | 0.4574372243184328 |
| 0.7857082349249467 | 0.4942381972086096 | 0.4909729232033229 |
| 0.8807137693372979 | 0.4120656014031141 | 0.5163726174160814 |
| 0.0941620203566558 | 0.4025316333004199 | 0.5013883336096328 |
| 0.2091627593371115 | 0.4758914699263954 | 0.4667702857624505 |
| 0.1181907705361525 | 0.5589184826560682 | 0.4454859455815807 |
| 0.8265980780651674 | 0.6307402283786487 | 0.4422612371952113 |
| 0.1703416929599442 | 0.3388384214442226 | 0.5176254964528937 |
| 0.2123336345040272 | 0.6155737825885552 | 0.4205555989445529 |
| 0.7433953764156485 | 0.3245084495440409 | 0.5711187277433112 |

S4

Comment

1.0000000000000000
6.4070494526731476 -0.0222975583821697 0.0155817754125660
-0.0520949819489813 14.9385140850697002 0.0566627806971775
-0.4315561987769719 0.0463190214024479 11.9984202843150172

O N C H Br
2 2 6 3 1

Direct

0.5129245367403570 0.5732496498801964 0.5714770780338725
0.4835457967498797 0.4028590981962950 0.3780914886008730
0.5675999458858314 0.5105192814358688 0.5077569993959088
0.4290529519191466 0.4621253767391167 0.4461789582125490
0.9051231172106640 0.5679843218901084 0.4569684401979472
0.7864455058469559 0.4944853646475096 0.4910682616170448
0.8820496677941492 0.4124393351803661 0.5165586163344784
0.0954581689230452 0.4029744851982073 0.5013770959356663
0.2100069043247359 0.4766951294013140 0.4657566559970405
0.1187227609876942 0.5598363415176024 0.4445025001413043
0.8266640621197467 0.6315356896529565 0.4418257893653603
0.1729402275336085 0.3394686749658860 0.5179864139134409
0.2128120735606700 0.6168121389117260 0.4192323057843268
0.7327997571526197 0.3154817597828554 0.5781400213297232

S5

Comment

1.0000000000000000
6.4794591913642252 -0.0100821735079856 0.0111439062861862
-0.0237515490716904 15.0639700967298058 0.0847376966420544
-0.4442306639999004 0.0680303418315193 11.7658889969533131

O N C H
2 3 6 5

Direct

0.5429529979767835 0.5983340835747839 0.5423747601077693
0.4957519611616519 0.3971670808127712 0.4057066649172825
0.7856747361371532 0.3513143508663745 0.5569901273083744
0.5924673208881472 0.5251339091360663 0.4986606066864567
0.4470563089449300 0.4685052759665211 0.4575434386429080
0.9305577875656539 0.5773544600402118 0.4555280468435541
0.8075171955021361 0.5046402088677482 0.4855834616182833
0.8976685745648325 0.4212229253259707 0.5147334056804169
0.1129318899427147 0.4143833762632667 0.5049985885041863
0.2315351949097746 0.4868946984770801 0.4740773813035304
0.1426835082472167 0.5699947523348783 0.4491408763568785
0.8540844314831304 0.6404533961282439 0.4376635422971873
0.1877200652144637 0.3505463949850807 0.5207356385738180
0.2365635833720106 0.6263810492958228 0.4250186995042498
0.8674574452907038 0.2942126675103509 0.5677016837538957
0.6458112237987095 0.3431946324148285 0.5134140649012124

S6

Comment

1.0000000000000000

| | | |
|---------------------|---------------------|---------------------|
| 6.4251186249469097 | -0.0246235563421653 | 0.0234282101274502 |
| -0.0574667770569036 | 15.0185781242200775 | 0.0804169295383118 |
| -0.4185751886115561 | 0.0661461059864522 | 11.9006161065407809 |

| | | | | |
|---|---|---|---|--|
| O | N | C | H | |
| 4 | 3 | 6 | 3 | |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.5463135210401546 | 0.5992805017930394 | 0.5465090307100979 |
| 0.5158892473898646 | 0.4036981438014422 | 0.3963042597357571 |
| 0.8554956763365098 | 0.2756688339586404 | 0.5364816278910496 |
| 0.6538713242840686 | 0.3697338407737334 | 0.6220580570154084 |
| 0.5987823840402200 | 0.5283324912945915 | 0.4981223143316669 |
| 0.4600175107961846 | 0.4728096103661983 | 0.4474202863104679 |
| 0.7962308866445227 | 0.3512046682371803 | 0.5585693698321705 |
| 0.9393536175256401 | 0.5816508714441113 | 0.4527924682371705 |
| 0.8169373199136345 | 0.5095299455539006 | 0.4861362366347137 |
| 0.9109707592044956 | 0.4270771009340493 | 0.5094289184828753 |
| 0.1225730606830311 | 0.4158314370787295 | 0.4948100899693628 |
| 0.2418680314736861 | 0.4891773858335640 | 0.4627187817651119 |
| 0.1529213711839859 | 0.5724948813867599 | 0.4421929908462587 |
| 0.8638053838171871 | 0.6452722991380995 | 0.4363258402805670 |
| 0.2480523761580784 | 0.6291825523614563 | 0.4180529704651477 |
| 0.1939603584605507 | 0.3512553587111711 | 0.5107042045554948 |

S7

Comment

| | | |
|---------------------|---------------------|---------------------|
| 1.0000000000000000 | | |
| 6.4147971655607430 | -0.0064394894666639 | 0.0116122540828592 |
| -0.0149411873291493 | 15.0092365779879096 | 0.0777390864929437 |
| -0.4391182385798514 | 0.0627085725436739 | 11.9277301197164949 |

| | | | | | |
|---|---|---|---|---|--|
| O | N | C | H | F | |
| 2 | 2 | 7 | 3 | 3 | |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.5439217514741657 | 0.5922918999379831 | 0.5624767074218937 |
| 0.5148091067858687 | 0.4190491613282532 | 0.3742515012348733 |
| 0.5970275422011397 | 0.5290033160963503 | 0.4996163670516225 |
| 0.4591980621846545 | 0.4806467034557613 | 0.4387723834213588 |
| 0.9319269962718764 | 0.5842709481311772 | 0.4476804311256899 |
| 0.8165431530545675 | 0.5111528736492730 | 0.4841641734632915 |
| 0.9140429588381096 | 0.4296827796486156 | 0.5111355430444462 |
| 0.1279046750765218 | 0.4221608875451537 | 0.4952641376350684 |
| 0.1455824749608254 | 0.5771256386648602 | 0.4347458355090197 |
| 0.2401962763515257 | 0.4951886147561524 | 0.4575847837278459 |
| 0.8087847781283486 | 0.3484691257731711 | 0.5604537400014209 |
| 0.8514508696119876 | 0.6470616185543889 | 0.4311270247678962 |
| 0.2366087554608924 | 0.6341330438212509 | 0.4077896133887151 |
| 0.2084377343765738 | 0.3597157629378671 | 0.5138481528099561 |
| 0.6216142639018543 | 0.3671173770237246 | 0.6056994049923929 |
| 0.9322966632314831 | 0.3126918472334310 | 0.6452425486082447 |
| 0.7769206444208407 | 0.2831049769092360 | 0.4836657505089690 |

S8

Comment

| | | |
|--------------------|---------------------|---------------------|
| 1.0000000000000000 | | |
| 6.4087306548907499 | -0.0000599669340153 | -0.0231485916949111 |

-0.0005886346520897 15.0953912739878859 0.0947195386935610
-0.5043199792937239 0.0767382701751532 11.8736420055364178

O N C H
3 2 7 6

Direct

0.5387464265701283 0.5867535394600125 0.5616284235904132
0.7802765790741404 0.3578172332171263 0.5562632486351546
0.5072716539989841 0.4065915354888929 0.3845659303830828
0.5927572471363334 0.5208740686196833 0.5035847929592734
0.4528154612272601 0.4690123054907076 0.4476416921980260
0.9304694517729004 0.5766499607213049 0.4552909897191668
0.8107251244671545 0.5044293263428656 0.4876882720685103
0.9038021750650458 0.4215641351539929 0.5139034461682002
0.1177615034535506 0.4117032496539821 0.4986529503762114
0.2336708639008762 0.4847597809673800 0.4652389178580165
0.1441669824010461 0.5678202370485863 0.4439489768089828
0.8666362287325171 0.2708963350291356 0.5722908234998982
0.8523750670451591 0.6399779147878277 0.4399907156126446
0.1970694468255445 0.3487446521942061 0.5136928082239436
0.2388936411842977 0.6239423482088782 0.4197802140714302
0.7388097051922955 0.2297189596823443 0.6012481262048652
0.9957670730988184 0.2706434622142595 0.6366527540801457
0.9211016058539343 0.2451676017188333 0.4925899365419966

S9

Comment

1.0000000000000000
6.4037918194723451 0.0010987803433640 -0.0064293528168257
0.0026148084336722 14.9815245091139762 0.0192262283038169
-0.4721096727163155 0.0153956299496592 11.9712861785956530

O N C H F
3 2 7 3 3

Direct

0.5505730218859455 0.5935764989340200 0.5548279412716255
0.7909896521955346 0.3644101697752831 0.5735189896041248
0.5230842111656884 0.3998732323330216 0.3982361592359780
0.6057196934324267 0.5235122749645100 0.5038706399282873
0.4672587950197595 0.4671153220810993 0.4538021172218833
0.9441988610225849 0.5764743783124544 0.4501304585448054
0.8244451193059845 0.5061369178022943 0.4893623653251566
0.9188706534946434 0.4253272002078461 0.5223648080231555
0.1322440000765113 0.4132541718701006 0.5101220244805305
0.1578851378570860 0.5661149022698027 0.4398235197639835
0.8307551797793451 0.2746381697136329 0.5685667986757892
0.2478037619161597 0.4841370788797121 0.4693019243888727
0.8664909514823194 0.6391769338647535 0.4286930515948981
0.2529498634446981 0.6205650101270450 0.4100683234406475
0.2104859762153737 0.3511166675729882 0.5333154720485851
0.6592951726888927 0.2325428702390369 0.6031524920035665
0.9959670210829614 0.2502642057788762 0.6377034665260126
0.8727111211360423 0.2466306022735196 0.4645547209766150

A10

Comment

1.0000000000000000
6.3924913679441575 -0.0034389757729352 -0.0070179532901847
-0.0078778492523737 15.1202104172411840 0.1451872642020784
-0.4726171317463562 0.1158574872535816 11.8835928867545011

O N C H
2 3 5 3

Direct

0.5203405424260339 0.5932110540672468 0.5406421825418022
0.4830032723360702 0.3843559038635362 0.4276561449663703
0.5725412869478177 0.5187648653581007 0.5015252986607237
0.4300785603742625 0.4573956900652760 0.4674981155544273
0.0946819435345319 0.4088549895757367 0.5078408259223295
0.9133138212532756 0.5734315765371107 0.4569833733526778
0.7912692878423968 0.5008664373573524 0.4876585963546773
0.8876919388254549 0.4190392058346504 0.5123373403518485
0.2081808453451757 0.4783961284871410 0.4777742805499514
0.1278578085995363 0.5623258849440020 0.4504460603159046
0.8390506128249200 0.6372581664867596 0.4398491311631858
0.7977316571320898 0.3613364975734896 0.5371957497485624
0.2285180691425452 0.6168969597829417 0.4269798810519703

A11

Comment

1.0000000000000000
6.2586434728772682 -0.0426526990868748 -0.0184026729661646
-0.1009767513492995 15.1598467013840494 0.1359306636238351
-0.4847974991314812 0.1124831958725266 12.1072907432300418

O N C H
2 4 4 2

Direct

0.5207880482789307 0.5782887155730876 0.5701227866345278
0.4817433528647470 0.3975147731846747 0.3996467875511129
0.5759931357923449 0.5132204697104186 0.5126049850538053
0.4334256084061252 0.4589462214998363 0.4619559347358049
0.0957059577164188 0.4142844647416979 0.5208493886914383
0.8859728447055133 0.4250705768716614 0.5297693611030851
0.9132312452755613 0.5728649409277367 0.4505064568575179
0.8009072423839427 0.5010833416285081 0.4945417548714204
0.2095180505224690 0.4798559481325952 0.4772606764267664
0.1300364099408924 0.5614809104185170 0.4408422869829707
0.8326985274578718 0.6339526170008014 0.4269196839507643
0.2338050916930143 0.6129703815104719 0.4083883863813469

A12

Comment

1.0000000000000000
6.3039281774194027 0.0014900857245692 0.0048412896088137
0.0044683820333283 15.1156656485751046 0.1417510615982240
-0.4437125116160552 0.1128886414504916 12.0532314440165322

O N C H
2 4 4 2

Direct

0.5191881688955107 0.5902316003150148 0.5488576704878341
0.4900674087716581 0.3891554311102894 0.4166978571368318

| | | |
|--------------------|--------------------|--------------------|
| 0.5746322350716895 | 0.5200413295223285 | 0.5020418876972030 |
| 0.4343202866795153 | 0.4591650973866095 | 0.4637895673570966 |
| 0.9098972329686958 | 0.5709146001921752 | 0.4540299884281822 |
| 0.0988787805485103 | 0.4081951706170486 | 0.5116693175419940 |
| 0.7987388663543129 | 0.5015271380100401 | 0.4880027958938342 |
| 0.8895122204492480 | 0.4193872479726863 | 0.5171281496384168 |
| 0.2100896332414308 | 0.4776030317132651 | 0.4777362475147839 |
| 0.1192441317482391 | 0.5597032717173107 | 0.4485407866896409 |
| 0.7955253715845387 | 0.3632234536812149 | 0.5445071057738247 |
| 0.2131450241200596 | 0.6158526277620240 | 0.4210639820735551 |

A13

Comment

| | | |
|---------------------|---------------------|---------------------|
| 1.0000000000000000 | | |
| 8.6062970473302673 | 0.0045893091379669 | 0.0144864272561501 |
| 0.1715990429406337 | 14.6286736153054608 | 0.0913522881059399 |
| -0.3147409830174180 | -0.3989587373870119 | 20.6519325064835151 |

| | | | |
|----|---|---|---|
| C | H | N | O |
| 10 | 6 | 2 | 2 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.7121433924810532 | 0.4691306599288438 | 0.4954216548279220 |
| 0.2878566075189468 | 0.5308693400711562 | 0.5045783151720755 |
| 0.7870981036369358 | 0.3821645629075689 | 0.4974442082091883 |
| 0.2129018963630642 | 0.6178354370924311 | 0.5025558207908105 |
| 0.7974066668433011 | 0.5488859573463429 | 0.4959020284627371 |
| 0.2025933331567060 | 0.4511140426536571 | 0.5040980015372654 |
| 0.9462866323332051 | 0.3764205230742022 | 0.5009573801680034 |
| 0.0537133786667923 | 0.6235795069257932 | 0.4990426198319966 |
| 0.0384419543797918 | 0.4563774666984344 | 0.5014305584239906 |
| 0.9615580226202098 | 0.5436225033015631 | 0.4985694415760094 |
| 0.7155271373493406 | 0.3214563641639288 | 0.4956550682394294 |
| 0.2844728626506594 | 0.6785436358360712 | 0.5043449317605706 |
| 0.7403502358072345 | 0.6153245677017551 | 0.4942348435761090 |
| 0.2596497641927655 | 0.3846754322982449 | 0.5057651564238910 |
| 0.0040324138717835 | 0.3097350245237394 | 0.5030428473560633 |
| 0.9959675881282166 | 0.6902649754762535 | 0.4969571526439367 |
| 0.5450854236958307 | 0.4653750028105037 | 0.4881915531757244 |
| 0.4549145763041693 | 0.5346249971894892 | 0.5118084468242756 |
| 0.4855472637020597 | 0.3946711166298726 | 0.4617242028645663 |
| 0.5144527362979332 | 0.6053288833701274 | 0.5382757971354266 |

A14

Comment

| | | |
|---------------------|---------------------|---------------------|
| 1.0000000000000000 | | |
| 23.3632030025608870 | 0.2732671814066319 | 0.0344100119374644 |
| 0.3162665543951116 | 15.7234619044918631 | -0.2898266051184536 |
| 0.3065534071320068 | -0.3733594499468004 | 19.9418690166592292 |

| | | | |
|----|----|---|---|
| C | H | N | O |
| 30 | 18 | 6 | 6 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.2523104539454098 | 0.4683110066353678 | 0.6808230320450914 |
| 0.7476895460397752 | 0.5316890231284503 | 0.3191769679498775 |
| 0.2435369393997713 | 0.4724164877322417 | 0.6107182513536592 |
| 0.7564630159190414 | 0.5275835122804132 | 0.3892817486413100 |

| | | |
|--------------------|--------------------|--------------------|
| 0.3068685184496098 | 0.4699870629395708 | 0.7054145289753382 |
| 0.6931314815741225 | 0.5300129072586270 | 0.2945854710196383 |
| 0.9561492109793366 | 0.4950923754077338 | 0.5790591114621729 |
| 0.0438507629456920 | 0.5049076245589705 | 0.4209409183563074 |
| 0.0046107816064555 | 0.4978067388868499 | 0.5353057294280066 |
| 0.9953891932344487 | 0.5021932610625094 | 0.4646942705669632 |
| 0.0609957153530100 | 0.4955941962768912 | 0.5600761965698186 |
| 0.9390043069955484 | 0.5044057739039894 | 0.4399237736519320 |
| 0.1070011403419980 | 0.4987852107172078 | 0.5155798074121521 |
| 0.8929988521902477 | 0.5012147892780948 | 0.4844201627593054 |
| 0.0983706817517702 | 0.5041053920613480 | 0.4455172054103052 |
| 0.9016293331500591 | 0.4958946377197931 | 0.5544828243578755 |
| 0.5422902156949957 | 0.5204539268466319 | 0.3589448093684667 |
| 0.4577098141206564 | 0.4795460732120089 | 0.6410551608532840 |
| 0.5518316511065154 | 0.5169196654980283 | 0.4289459893079225 |
| 0.4481683787101032 | 0.4830803344972824 | 0.5710539808635362 |
| 0.5879234141272903 | 0.5240144471736474 | 0.3149300301464922 |
| 0.4120765858859249 | 0.4759855826075221 | 0.6850699996719886 |
| 0.2894197154302229 | 0.4764323695062501 | 0.5662310254716342 |
| 0.7105803143550116 | 0.5235676006459812 | 0.4337690043468456 |
| 0.3459157948594191 | 0.4771095427388368 | 0.5910985381250233 |
| 0.6540842349403378 | 0.5228904274593589 | 0.4089014618699453 |
| 0.3551112601784115 | 0.4743944651958943 | 0.6617841009431114 |
| 0.6448887099835044 | 0.5256055050023024 | 0.3382158990518579 |
| 0.3932468908185514 | 0.4818080014265877 | 0.5460857425780025 |
| 0.6067531092091741 | 0.5181920284005322 | 0.4539142574169662 |
| 0.3135001403675981 | 0.4678078518670291 | 0.7593219382696945 |
| 0.6864998894273696 | 0.5321921480909924 | 0.2406780766118837 |
| 0.9627990261927040 | 0.4917675708127778 | 0.6328901555881866 |
| 0.0372010297242241 | 0.5082324291539051 | 0.3671098741800015 |
| 0.0675159709259811 | 0.4914131832421300 | 0.6135607239203046 |
| 0.9324840439857602 | 0.5085867869560599 | 0.3864392760746575 |
| 0.1357206938230691 | 0.5081001233286372 | 0.4127115202300923 |
| 0.8642792912437171 | 0.4918998766666660 | 0.5872884499413669 |
| 0.5804944868682826 | 0.5258973685362597 | 0.2611642350697292 |
| 0.4195055429334646 | 0.4741026314764021 | 0.7388357649252405 |
| 0.2829781767717306 | 0.4794596598420341 | 0.5126739895844397 |
| 0.7170218828469325 | 0.5205403103561552 | 0.4873260104105304 |
| 0.3857056950176846 | 0.4846015695031592 | 0.4927289741974080 |
| 0.6142942751730009 | 0.5153984007236577 | 0.5072709662008389 |
| 0.5016184649758366 | 0.4792038310633232 | 0.6582334702024475 |
| 0.4983815350370179 | 0.5207961987811410 | 0.3417665596160324 |
| 0.7849171135281677 | 0.5365006433033063 | 0.2862777834260122 |
| 0.2150828715666566 | 0.4634993567093483 | 0.7137222165689571 |
| 0.1843552334210266 | 0.4665872691442042 | 0.5914223445279696 |
| 0.8156447665617991 | 0.5334127308684509 | 0.4085776554670007 |
| 0.1662314199537493 | 0.5034733405717232 | 0.5347805673994350 |
| 0.8337685800171686 | 0.4965266892094182 | 0.4652194623687608 |
| 0.4998994924106779 | 0.5177774156154101 | 0.4695347916560672 |
| 0.5001005075721485 | 0.4822225843972447 | 0.5304652083389024 |
| 0.1497687232596999 | 0.4298558979033850 | 0.6301073648377753 |
| 0.8502312916514375 | 0.5701440722948330 | 0.3698926352074870 |
| 0.2009126995167998 | 0.5399092689495636 | 0.4960573490775912 |
| 0.7990873302867015 | 0.4600907608142900 | 0.5039426509676709 |

| | | |
|--------------------|--------------------|--------------------|
| 0.4541060768947791 | 0.5494034208934102 | 0.4454538498580699 |
| 0.5458939529218386 | 0.4505965791019012 | 0.5545461203133957 |

A15

Comment

| | | |
|---------------------|---------------------|---------------------|
| 1.000000000000000 | | |
| 13.1980026399157317 | -0.0047538950779796 | -0.0309734467705216 |
| 0.1107892569213019 | 16.4378674838848013 | -0.1326262866383477 |
| 0.1223418097334811 | -0.4035514074766560 | 19.8497887903268229 |

| | | | |
|----|----|---|---|
| C | H | N | O |
| 20 | 12 | 4 | 4 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.3633987788374426 | 0.4589089315926103 | 0.6468470669551891 |
| 0.2585842714045441 | 0.4719034319525974 | 0.6390841113711474 |
| 0.4284203581025565 | 0.4658586010592600 | 0.5928768160678004 |
| 0.4171475391630395 | 0.5129434134224198 | 0.4088312047081573 |
| 0.3124751807398027 | 0.5267176950547920 | 0.4011726015094581 |
| 0.4541404240598013 | 0.4930409059918759 | 0.4710090075412623 |
| 0.2210163886980041 | 0.4937449917650270 | 0.5774574157540400 |
| 0.2842389579868083 | 0.5012930526620565 | 0.5197824654872392 |
| 0.3907107188336951 | 0.4862069455996760 | 0.5286402167914446 |
| 0.2474462371104238 | 0.5213331694728467 | 0.4553618336269736 |
| 0.8770292384030540 | 0.4380194236508999 | 0.4210449999438879 |
| 0.7720852582259070 | 0.4540798945506239 | 0.4220565031426347 |
| 0.9409617662948193 | 0.4792778036529910 | 0.4646412686301673 |
| 0.9260483987180876 | 0.6437959284368517 | 0.6000812158875348 |
| 0.8210027403985833 | 0.6594376534876147 | 0.6013816470128006 |
| 0.9648540472020528 | 0.5843694575840459 | 0.5567689066856971 |
| 0.7337635449433009 | 0.5122615001554749 | 0.4665827337075470 |
| 0.7960498660525275 | 0.5570352701231300 | 0.5125168942875717 |
| 0.9027744139899312 | 0.5390387929172675 | 0.5110602340132857 |
| 0.7570533115721929 | 0.6170966298995566 | 0.5585540646068381 |
| 0.5090284474253579 | 0.4537500614789636 | 0.5986701418551519 |
| 0.1671324563973755 | 0.5336704757435271 | 0.4486556639988208 |
| 0.4687269135818681 | 0.5186465049583333 | 0.3663453713139688 |
| 0.3927582967994638 | 0.4426609534916821 | 0.6959036820778124 |
| 0.2831119223024956 | 0.5424307634071539 | 0.3519854953640902 |
| 0.2061805798410390 | 0.4646948589725923 | 0.6809416302020850 |
| 0.0215180468547658 | 0.4649450146287393 | 0.4639152376000126 |
| 0.6762945794462496 | 0.6308691669897897 | 0.5584854038254790 |
| 0.9776024936468062 | 0.6780954972393829 | 0.6326017729317925 |
| 0.9074506968462472 | 0.3920346864925222 | 0.3857885548504569 |
| 0.7906382568054795 | 0.7058872109399701 | 0.6362406615719536 |
| 0.7213743280806781 | 0.4206180659915901 | 0.3883813893212036 |
| 0.1117629708989796 | 0.5021510200168109 | 0.5737357558664939 |
| 0.0741917145573510 | 0.5750406482078247 | 0.5570886658316425 |
| 0.6269587769646350 | 0.5329816172815285 | 0.4642038281990679 |
| 0.5608246893404214 | 0.4735898233460105 | 0.4778697610266178 |
| 0.0547969484982787 | 0.4442781870997692 | 0.5915784835682345 |
| 0.1310194481103295 | 0.6360493532653706 | 0.5476592068039636 |
| 0.5987042638608031 | 0.6046084487292589 | 0.4498424664428455 |
| 0.5888927532779249 | 0.4033741059281724 | 0.4961558575931448 |

A16

Comment

1.0000000000000000
10.8538081026000999 -0.0022923460349089 -0.0091491699034564
-0.0041081058677290 19.5107130762342607 0.0979964388014859
-0.0167127742282756 0.0998358029473032 20.0226608749220460

C H N O
14 8 2 2

Direct

0.1669065615890446 0.4570587412435430 0.3992029848280367
0.8330934384109554 0.5429412587564570 0.6007970151719633
0.0811395437747962 0.4779401718012011 0.4489695867525967
0.9188604562252038 0.5220598281987989 0.5510304132474104
0.9537910155873206 0.4710846797356112 0.4409166367839177
0.0462089844126794 0.5289153502643842 0.5590833632160823
0.1288529534942384 0.5074777947130329 0.5096295534244248
0.8711470465057616 0.4925222052869671 0.4903704465755752
0.7416721782690630 0.4860181399259389 0.4814328710506359
0.2583278217309370 0.5139818600740611 0.5185671289493712
0.6627040803505793 0.5070289702157140 0.5311715018913858
0.3372959196494207 0.4929710297842860 0.4688284981086142
0.7089585555257827 0.5352173985888982 0.5918209446166358
0.2910414444742173 0.4647826014111018 0.4081790553833642
0.1317463661747382 0.4347271259069672 0.3532252183160622
0.8682536338252618 0.5652728450930411 0.6467747816839378
0.9175512427426469 0.4488253676101408 0.3950873920879943
0.0824487572573531 0.5511746323898521 0.6049126379120082
0.7066937871218357 0.4645337945275472 0.4354019933333575
0.2933062128781643 0.5354662054724528 0.5645980066666425
0.6430984213171484 0.5497831334448833 0.6299661452109788
0.3569015786828516 0.4502168665551167 0.3700338547890212
0.5306093987035467 0.4988275339932571 0.5296359172373784
0.4693906012964533 0.5011724660067429 0.4703640827626216
0.5268456163933521 0.5074260130968824 0.4151388058310346
0.4731543836066479 0.4925739869031176 0.5848611941689654

A17

Comment

1.0000000000000000
10.8194481084669452 -0.0148072339435574 -0.0078937334795746
-0.0146283234540755 11.8066854183551975 -0.0491394726630052
-0.0064889519757082 -0.0499908153816326 11.6111523497050833

O N C H
2 2 12 8

Direct

0.5305781975016259 0.6400646547979321 0.4644472392333512
0.5201035357879817 0.3578782552568569 0.5384207526931775
0.5630933799483557 0.5411184631198722 0.4947494166573705
0.4808066889920042 0.4569586909268537 0.5160916195970771
0.7663437403448512 0.5765779534342670 0.4213010344665591
0.6939430989992204 0.5163967643424670 0.4998135693243029
0.7493314602067969 0.4471014029249432 0.5822851614972251
0.8776155896998858 0.4393683687980641 0.5852133858567967
0.9524922235049544 0.4980013334701638 0.5065803318868305
0.8939417941721928 0.5662203106083439 0.4241723892727478

| | | |
|--------------------|--------------------|--------------------|
| 0.1622240631978542 | 0.5842624718547782 | 0.4839168809481222 |
| 0.0883020787129496 | 0.4901309624167993 | 0.5102933310761415 |
| 0.1488319873336437 | 0.3890102680609999 | 0.5396438201962539 |
| 0.2767326906842342 | 0.3821096360719594 | 0.5407699587163819 |
| 0.3491273853453549 | 0.4773182373146838 | 0.5133440640614992 |
| 0.2906970527607626 | 0.5797700282638161 | 0.4852089624901410 |
| 0.7207267886398796 | 0.6309664605023073 | 0.3592979608057050 |
| 0.6933897926020336 | 0.4009900928173451 | 0.6437023377564088 |
| 0.9206958311993318 | 0.3882606106972517 | 0.6518287598299253 |
| 0.9492769170760980 | 0.6105200426591395 | 0.3603656137449747 |
| 0.1183967128760770 | 0.6646951473304696 | 0.4636709798613836 |
| 0.0946645711678755 | 0.3135705648740768 | 0.5589968275307555 |
| 0.3235290378645317 | 0.3035253272823866 | 0.5614308036573235 |
| 0.3444753393815034 | 0.6542337611742397 | 0.4649547808395482 |

A18

Comment

| | | |
|---------------------|---------------------|---------------------|
| 1.0000000000000000 | | |
| 13.2024043934759856 | -0.0794499362814162 | 0.1672592102285220 |
| -0.1335228557901959 | 20.3227249737120168 | -0.5539349446825004 |
| 0.2203742939779705 | -0.3650366647644300 | 19.5116484901359648 |

| | | | |
|----|----|---|---|
| C | H | N | O |
| 18 | 10 | 2 | 2 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.6598191790044083 | 0.5425436697822477 | 0.5929148828209705 |
| 0.7372697389315235 | 0.5181961330648264 | 0.5463422166917908 |
| 0.7800285460961192 | 0.4583042572967315 | 0.4374660803170869 |
| 0.7061693418573043 | 0.4832244524990870 | 0.4838279183986103 |
| 0.6011146619734902 | 0.4746289725211597 | 0.4703097508219685 |
| 0.5293666281607443 | 0.4988567414416778 | 0.5172507676945699 |
| 0.5595865618407672 | 0.5330487692933588 | 0.5795364511477743 |
| 0.8840636895084018 | 0.4664196566618131 | 0.4498326801091679 |
| 0.8399887632958567 | 0.5267278739417023 | 0.5589421678666042 |
| 0.9151426633605055 | 0.5018610079374355 | 0.5124302613519021 |
| 0.1394654457467865 | 0.4251958871981429 | 0.3697690174226977 |
| 0.1980888520267428 | 0.4935725803874789 | 0.4921325723036034 |
| 0.2698356434330051 | 0.4690328915936988 | 0.4453851621671632 |
| 0.2396718733832159 | 0.4345779969446255 | 0.3832488609941791 |
| 0.9592612313279147 | 0.4414063787182059 | 0.4034446717796172 |
| 0.0619700606916354 | 0.4498897941770750 | 0.4161145508114927 |
| 0.0191514107437314 | 0.5100054089828348 | 0.5248399826357613 |
| 0.0930494379695546 | 0.4850276134495388 | 0.4785479242701172 |
| 0.6821210608509887 | 0.5691480604513401 | 0.6400831248554724 |
| 0.7563594584809721 | 0.4318874231737695 | 0.3904551136477608 |
| 0.5790331747714674 | 0.4487152006740942 | 0.4231822770044218 |
| 0.5004839814737210 | 0.5505973565488844 | 0.6152519881256069 |
| 0.8633503298499221 | 0.5531600783402340 | 0.6060325944886742 |
| 0.1171888338013503 | 0.3983673792932763 | 0.3227209815489545 |
| 0.2201641167850497 | 0.5196307968248632 | 0.5391859338547462 |
| 0.2987911465840085 | 0.4167033513921439 | 0.3477175484701434 |
| 0.9359510187240758 | 0.4148129127741669 | 0.3564306349855997 |
| 0.0427581129209997 | 0.5364031212320626 | 0.5718773855565047 |
| 0.4212194580127928 | 0.4900017142849649 | 0.5123615157858126 |
| 0.3779763501080922 | 0.4778264957389950 | 0.4503103294125026 |

| | | |
|--------------------|--------------------|--------------------|
| 0.3666680535429307 | 0.4961571905478834 | 0.5670404805770346 |
| 0.4324512487419270 | 0.4716787228317045 | 0.3956142190816649 |

DIMERS

1-dim

Comment

| | | |
|---------------------|---------------------|---------------------|
| 1.0000000000000000 | | |
| 20.0000000000000000 | 0.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 20.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 15.0000000000000000 |

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|----|---|----|---|
| C | O | H | N |
| 12 | 2 | 10 | 2 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.4072536370893609 | 0.5141850379934423 | 0.5087760505968745 |
| 0.3793190379123451 | 0.4848242410343172 | 0.5843009361533805 |
| 0.3107569817418614 | 0.4722336070579765 | 0.5855112700333343 |
| 0.2712618462947675 | 0.4890543734410103 | 0.5120067789401820 |
| 0.3003087995129516 | 0.5184020875095589 | 0.4368664320352532 |
| 0.3688700398965020 | 0.5312243455247478 | 0.4347857730522020 |
| 0.5917147192187949 | 0.4962157147155011 | 0.4875086369410559 |
| 0.6297916570912688 | 0.4373696660456272 | 0.4883415295335122 |
| 0.6225103016356731 | 0.5591553376400080 | 0.4897513514106379 |
| 0.6990717752425060 | 0.4415754406332764 | 0.4943005244137497 |
| 0.6921354357001859 | 0.5621829736530473 | 0.4945512877447900 |
| 0.7305112069182927 | 0.5039585526250498 | 0.4978377792156506 |
| 0.4940436037989166 | 0.5895139660628247 | 0.5435195103925170 |
| 0.4970429090982394 | 0.4310603292075241 | 0.4525979154639993 |
| 0.4109954847483854 | 0.4722905905854919 | 0.6409479797381116 |
| 0.2881644046644853 | 0.4494190825791479 | 0.6442303987222948 |
| 0.2694705624030014 | 0.5315934301098079 | 0.3795949306121519 |
| 0.3924583538825404 | 0.5540606080451776 | 0.3768625614775742 |
| 0.6039478649569527 | 0.3896229919460812 | 0.4842087330978764 |
| 0.5927945934776260 | 0.6044428310121829 | 0.4881745048688673 |
| 0.7286403995756718 | 0.3958187833720808 | 0.4960884019152615 |
| 0.7163385785433779 | 0.6109943678075335 | 0.4961528944355162 |
| 0.2176164376546513 | 0.4794351129241734 | 0.5134528783292978 |
| 0.7848147666590846 | 0.5071148771845508 | 0.5028721834996216 |
| 0.4775648399290653 | 0.5329893946966627 | 0.5115338071771919 |
| 0.5203317503534891 | 0.4861622285932221 | 0.4816849711991094 |

S2-dim

Comment

| | | |
|---------------------|---------------------|---------------------|
| 1.0000000000000000 | | |
| 20.0000000000000000 | 0.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 20.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 15.0000000000000000 |

| | | | | |
|----|---|---|---|---|
| C | O | H | F | N |
| 12 | 2 | 8 | 2 | 2 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.4085518352282157 | 0.5136043238188479 | 0.5228067739456148 |
| 0.3731076454615070 | 0.4933327073355939 | 0.5984526674951774 |
| 0.3049988230239460 | 0.4809584067822448 | 0.5917380276024092 |
| 0.2721007668109882 | 0.4896076165688110 | 0.5105935151468691 |

| | | |
|--------------------|--------------------|--------------------|
| 0.3066157775982650 | 0.5113970848892493 | 0.4354403824963707 |
| 0.3747695621639480 | 0.5233287822029016 | 0.4426025722239967 |
| 0.5901895835389762 | 0.4965242595815234 | 0.4879390506213639 |
| 0.6280875174777532 | 0.4380256899889385 | 0.4848084850759747 |
| 0.6198945010868673 | 0.5596217224462707 | 0.4860275522617203 |
| 0.6972720673630456 | 0.4420800569896987 | 0.4893676327126140 |
| 0.6892633277414264 | 0.5603806857343742 | 0.4783617297130265 |
| 0.7290545520488508 | 0.5038538163992631 | 0.4882396669191462 |
| 0.5002549672344639 | 0.5695085377896504 | 0.5874951161869606 |
| 0.4952570717317932 | 0.4412390624756920 | 0.4343330078413629 |
| 0.2772016900826923 | 0.4641334106747475 | 0.6505585373316739 |
| 0.2814845046139758 | 0.5193249880082957 | 0.3721137934173359 |
| 0.6026640973318069 | 0.3903996899207317 | 0.4791171067783156 |
| 0.5904254091557324 | 0.6049804491964209 | 0.4879255272751396 |
| 0.7275782831106272 | 0.3970180018710350 | 0.4883042343022175 |
| 0.4001193039773606 | 0.4875803862278383 | 0.6608025151014508 |
| 0.2185436775544065 | 0.4795890686616393 | 0.5053861680816746 |
| 0.7831961104892801 | 0.5089986335954261 | 0.4909504630629418 |
| 0.4095639219451658 | 0.5455772126789702 | 0.3713677155637803 |
| 0.7209796542861941 | 0.6197632670840156 | 0.4599202178642318 |
| 0.4789310185120583 | 0.5270553248004455 | 0.5309363319985716 |
| 0.5189844064306691 | 0.4880567562773488 | 0.4820712619800531 |

S3-dim

Comment

| | | |
|---------------------|---------------------|---------------------|
| 1.0000000000000000 | | |
| 20.0000000000000000 | 0.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 20.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 15.0000000000000000 |

| | | | | | |
|----|---|---|----|---|--|
| C | O | H | Cl | N | |
| 12 | 2 | 8 | 2 | 2 | |

Direct

| | | |
|---------------------|--------------------|--------------------|
| 0.4079457090071728 | 0.5098727308687359 | 0.5232540577948441 |
| 0.3707829721564693 | 0.4953233934869488 | 0.5994754057087803 |
| 0.3020997508178169 | 0.4851710243455116 | 0.5926893632616270 |
| 0.2707803773982320 | 0.4903645284261771 | 0.5096976626109253 |
| 0.30770513766615358 | 0.5062298740806881 | 0.4337140161059452 |
| 0.3765937722117769 | 0.5164085181761706 | 0.4401723197594194 |
| 0.5918272074631190 | 0.4923688728610998 | 0.4953679616520930 |
| 0.6308471453633899 | 0.4367406248846564 | 0.4724853781744827 |
| 0.6209962523113290 | 0.5550044892035828 | 0.5110583626475460 |
| 0.6998865695564689 | 0.4438737542591724 | 0.4664680715911942 |
| 0.6902750309877916 | 0.5604402119394649 | 0.5033104018000572 |
| 0.7303697251612107 | 0.5055937290906556 | 0.4818721769386443 |
| 0.4959682050142504 | 0.5731311523275409 | 0.5839072852480953 |
| 0.4969267215413282 | 0.4283803874020791 | 0.4596043994307806 |
| 0.2730881161325627 | 0.4733027739658198 | 0.6520750815892811 |
| 0.2836354946831108 | 0.5112354002043347 | 0.3689414748216180 |
| 0.6060095619572579 | 0.3894481725017513 | 0.4591379666357369 |
| 0.5910007418492853 | 0.5980979466859040 | 0.5289217013814351 |
| 0.7305476015033676 | 0.4007244614123024 | 0.4492181788331848 |
| 0.3965817427288130 | 0.4923433518610381 | 0.6632999463698681 |
| 0.7843811502037425 | 0.5114618455941624 | 0.4773230489550429 |
| 0.2170230160595068 | 0.4825179032964115 | 0.5038509324908844 |

| | | |
|--------------------|--------------------|--------------------|
| 0.4216835784343758 | 0.5382258608661559 | 0.3468609822647508 |
| 0.7271850839772398 | 0.6376510532861417 | 0.5213638669940792 |
| 0.4783712353741194 | 0.5244059905058123 | 0.5347289818018552 |
| 0.5206681404447195 | 0.4804820084676606 | 0.4963309331378198 |

S4-dim

Comment

| | | |
|---------------------|---------------------|---------------------|
| 1.0000000000000000 | | |
| 20.0000000000000000 | 0.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 20.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 15.0000000000000000 |

| | | | | |
|----|---|---|----|---|
| C | O | H | Br | N |
| 12 | 2 | 8 | 2 | 2 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.4070676925848489 | 0.5114108088191068 | 0.5169897447153223 |
| 0.3762331964353670 | 0.4811357106526699 | 0.5898911876647419 |
| 0.3077588346405173 | 0.4685158573130560 | 0.5874328162141454 |
| 0.2705368883520538 | 0.4867450412176929 | 0.5124784868876611 |
| 0.3013734891806267 | 0.5173741144478690 | 0.4396820859500200 |
| 0.3699923419868679 | 0.5297456259048720 | 0.4419730035308537 |
| 0.5908575864416895 | 0.4945848490017512 | 0.4924051792160398 |
| 0.6303876174811116 | 0.4368636357053506 | 0.4941786373309230 |
| 0.6192023354234550 | 0.5585433873195249 | 0.4890529462524216 |
| 0.6996524025096390 | 0.4434888693543255 | 0.4947661683369166 |
| 0.6887224996807919 | 0.5630969165091164 | 0.4882666945005101 |
| 0.7295634465527293 | 0.5065763559481954 | 0.4919494015355340 |
| 0.4945395538402602 | 0.5820943009626169 | 0.5639828728306124 |
| 0.4964882396533420 | 0.4296813348781175 | 0.4561488141293311 |
| 0.2835247438901157 | 0.4445444018371664 | 0.6440716820708400 |
| 0.2725994031343674 | 0.5318579528611780 | 0.3811652015105492 |
| 0.6060252160865313 | 0.3882551947920924 | 0.4944599002443856 |
| 0.5882005694353867 | 0.6030238199349195 | 0.4873567204130413 |
| 0.7309981130765156 | 0.3989406429420904 | 0.4971910700578641 |
| 0.4064171094675743 | 0.4677324830037986 | 0.6476393758565924 |
| 0.2169020954982977 | 0.4772933645583692 | 0.5103540321407313 |
| 0.7837312012612387 | 0.5119057609541412 | 0.4923414499040740 |
| 0.4124206589449242 | 0.5712892254069073 | 0.3435385442464837 |
| 0.7288338539590627 | 0.6492842576089828 | 0.4824547149678338 |
| 0.4773660940227058 | 0.5287884185804470 | 0.5240049894410531 |
| 0.5196348154600433 | 0.4834176144856541 | 0.4893042410515480 |

S5-dim

Comment

| | | |
|---------------------|---------------------|---------------------|
| 1.0000000000000000 | | |
| 20.0000000000000000 | 0.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 20.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 15.0000000000000000 |

| | | | |
|----|---|----|---|
| C | O | H | N |
| 12 | 2 | 12 | 4 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.4062768407783048 | 0.5188852770216024 | 0.5088002921299091 |
| 0.3791528724111271 | 0.4857769403844796 | 0.5821549807988188 |
| 0.3116803560784413 | 0.4693003565585661 | 0.5833131726152071 |
| 0.2723424049566557 | 0.4851782540068940 | 0.5089796977482834 |

| | | |
|--------------------|--------------------|--------------------|
| 0.2991072227516768 | 0.5190755795349473 | 0.4365060168314275 |
| 0.3668816848655115 | 0.5383519403532083 | 0.4349993060552642 |
| 0.5919926383092554 | 0.4940355303703846 | 0.5007800006330323 |
| 0.6286454224151430 | 0.4341535558493067 | 0.5022031432832957 |
| 0.6241474491235832 | 0.5560437244513369 | 0.4940755283070498 |
| 0.6978783633060357 | 0.4375685925030673 | 0.4986537123192668 |
| 0.6943776368550133 | 0.5584252789322265 | 0.4898011854008758 |
| 0.7309458666280397 | 0.4987367894953217 | 0.4930580259153714 |
| 0.4935452984566447 | 0.5966555089139366 | 0.4904397075231835 |
| 0.4976316253346342 | 0.4254848284343877 | 0.5181166689918467 |
| 0.2901359320503868 | 0.4434760693795570 | 0.6404710361683709 |
| 0.2677346755723157 | 0.5309756114871053 | 0.3790893727701451 |
| 0.6021353193978546 | 0.3869107241303305 | 0.5058215932313392 |
| 0.5956532708231964 | 0.6019824470647686 | 0.4952072693650050 |
| 0.7267724976326639 | 0.3914591450144132 | 0.4982473766190341 |
| 0.4117892494962971 | 0.4721271933585526 | 0.6371883429434358 |
| 0.3624226737453149 | 0.5898685368109579 | 0.3174709111101006 |
| 0.4351697699426992 | 0.5999177416329768 | 0.3768935787906630 |
| 0.7103662087353295 | 0.6536609364075127 | 0.4417235483860481 |
| 0.7771847384536613 | 0.6190461596769684 | 0.4924851595211406 |
| 0.2197837270664847 | 0.4709286075903714 | 0.5078163669926574 |
| 0.7853461646185697 | 0.5003977538574145 | 0.4892849842140704 |
| 0.3945748843855544 | 0.5709705885711078 | 0.3630951739313369 |
| 0.4763927345152206 | 0.5358483749318432 | 0.5053166967042286 |
| 0.5201985802839278 | 0.4842873938546327 | 0.5081756101850862 |
| 0.7265339230104571 | 0.6206004774218228 | 0.4883515545144966 |

S6-dim

Comment

| | | |
|---------------------|---------------------|---------------------|
| 1.0000000000000000 | | |
| 20.0000000000000000 | 0.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 20.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 15.0000000000000000 |

| C | O | H | N |
|----|---|---|---|
| 12 | 6 | 8 | 4 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.4077807704831081 | 0.5136360140072248 | 0.5124535017467767 |
| 0.3787630441740760 | 0.4846615985942215 | 0.5874558715724458 |
| 0.3104319315028231 | 0.4712459122208459 | 0.5888603440814882 |
| 0.2707043073137866 | 0.4875591855468557 | 0.5154014547208383 |
| 0.2994735304501757 | 0.5169517153707386 | 0.4405215066203342 |
| 0.3680241052525978 | 0.5298959877929098 | 0.4386924888146089 |
| 0.5908833776477314 | 0.4952680881427606 | 0.4918011817631242 |
| 0.6293949827929863 | 0.4367783578366293 | 0.4912454220347728 |
| 0.6206120997690813 | 0.5584398418611558 | 0.4920223162838422 |
| 0.6987951451549059 | 0.4414792958177972 | 0.4947922881309375 |
| 0.6901229376676909 | 0.5608798052967287 | 0.4931243046912671 |
| 0.7299822099864376 | 0.5037959433487490 | 0.4963109079862242 |
| 0.4944962946600074 | 0.5839546703405466 | 0.5613037561637082 |
| 0.4957740947551220 | 0.4329625399921707 | 0.4508858510223361 |
| 0.3576836262656767 | 0.5738226151384745 | 0.2959939831027030 |
| 0.4576301384784492 | 0.5709951672611734 | 0.3562717485038188 |
| 0.6868741595478877 | 0.6769835867155689 | 0.4836618590950252 |
| 0.7851267728954976 | 0.6280067168175072 | 0.4910912646501124 |

| | | |
|--------------------|--------------------|--------------------|
| 0.2882732093448366 | 0.4482170086091258 | 0.6476997915769235 |
| 0.2699178213571711 | 0.5304999028528532 | 0.3824441491102419 |
| 0.6039107748166005 | 0.3888341003900775 | 0.4874539308896562 |
| 0.5915658851242529 | 0.6041364281926218 | 0.4905925425917987 |
| 0.7288828880854773 | 0.3960934590505668 | 0.4957499385496419 |
| 0.4104931631675974 | 0.4729377232069636 | 0.6442843674982877 |
| 0.2171394439062972 | 0.4776540933674561 | 0.5166900005667248 |
| 0.7840422052740639 | 0.5090488460935623 | 0.4992776218807869 |
| 0.3965662879058983 | 0.5604225727940363 | 0.3576644000617364 |
| 0.4780401591703478 | 0.5312780393571573 | 0.5198716312631194 |
| 0.5198343126644375 | 0.4854734585445197 | 0.4867504882591582 |
| 0.7231602773849629 | 0.6270273474389860 | 0.4892711797675596 |

S7-dim

Comment

| | | |
|---------------------|---------------------|---------------------|
| 1.0000000000000000 | | |
| 20.0000000000000000 | 0.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 20.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 15.0000000000000000 |

| C | O | F | H | N |
|----|---|---|---|---|
| 14 | 2 | 6 | 8 | 2 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.4070603988017037 | 0.5081898726823382 | 0.5098085820904237 |
| 0.3762377278742146 | 0.4791982358776751 | 0.5836385044543436 |
| 0.3070784147419179 | 0.4706599684078993 | 0.5843978268407523 |
| 0.2689288743398376 | 0.4910544309290827 | 0.5113148601157507 |
| 0.3000921443031199 | 0.5192198869615969 | 0.4371807688308987 |
| 0.3694876077763152 | 0.5283435446974818 | 0.4354296449547794 |
| 0.5928038222085500 | 0.4924740722195543 | 0.4947485005684537 |
| 0.6337203382063993 | 0.4356174372084217 | 0.4950432419431978 |
| 0.6203537858790069 | 0.5568862835233764 | 0.4934951524907114 |
| 0.7029963324298338 | 0.4428972108871208 | 0.4942655626565042 |
| 0.6898529322731016 | 0.5627681792219817 | 0.4917089633054525 |
| 0.7313339593943170 | 0.5064770144519106 | 0.4917386325788075 |
| 0.4010816648585470 | 0.5583091515950324 | 0.3531828846982665 |
| 0.7223428908987146 | 0.6306147884148083 | 0.4876500866175453 |
| 0.4929890203024739 | 0.5790637996486061 | 0.5594249481223024 |
| 0.5004353846198257 | 0.4237076621951370 | 0.4610841662923807 |
| 0.3550375847821041 | 0.5908084896889833 | 0.3017812105317362 |
| 0.4500201464387266 | 0.6036071823035345 | 0.3729111483069475 |
| 0.4298207451488520 | 0.5105538657897213 | 0.3003255164578117 |
| 0.6811515703063655 | 0.6805548311376322 | 0.5157765501168342 |
| 0.7788523085603043 | 0.6329764724272515 | 0.5392952984599237 |
| 0.7418251583380358 | 0.6461091166323224 | 0.4025919323764446 |
| 0.2829561090004988 | 0.4488840371706280 | 0.6427974150642597 |
| 0.2705539518731777 | 0.5354988516534854 | 0.3802129650479408 |
| 0.6102325146510357 | 0.3865511645411757 | 0.4961455003258352 |
| 0.5887166818749587 | 0.6009709138257517 | 0.4942719322433565 |
| 0.7351094623861445 | 0.3988640931402426 | 0.4959597690398551 |
| 0.4067936909308702 | 0.4644499409054377 | 0.6403962272355290 |
| 0.2147019391436771 | 0.4856715181450516 | 0.5121663411158475 |
| 0.7854143695022503 | 0.5129158613767512 | 0.4905524186943741 |
| 0.4777309555785916 | 0.5253529489005097 | 0.5192686550207523 |
| 0.5217375225765112 | 0.4793691444395145 | 0.4905747484019755 |

S8-dim

Comment

```
1.00000000000000000000
20.000000000000000000 0.000000000000000000 0.000000000000000000
0.00000000000000000000 20.000000000000000000 0.000000000000000000
0.00000000000000000000 0.000000000000000000 15.000000000000000000
```

```
C      O      H      N
14      4      14      2
```

Direct

```
0.4114376399371559 0.5184748081567084 0.5128413621988429
0.3785070833504622 0.4910092803557773 0.5856768650536919
0.3104156302588071 0.4762709517834829 0.5801133048150359
0.2762390268653516 0.4894809369130738 0.5009751489575400
0.3089834336040635 0.5183949258922956 0.4282056063611255
0.3772134445534690 0.5337643244513960 0.4334813369587232
0.5947282045618633 0.4951970398663573 0.4900681647588288
0.6306160189718988 0.4353001808461102 0.4877524116468175
0.6267765447797335 0.5574025310764990 0.4949634856342469
0.7001510587235527 0.4379502123782178 0.4939646806417593
0.6965705316106133 0.5585923964431059 0.5008454218324462
0.7332902040537608 0.4988321621379642 0.5015126227612557
0.3809468972779973 0.5750610782009864 0.2840402579887113
0.6982284631715330 0.6780465637183877 0.5024185425447709
0.5016895941552904 0.5828879626827048 0.5682037074874527
0.4977591054836064 0.4379860327245462 0.4439409149498403
0.4136192175922093 0.5629343192337876 0.3673780798416212
0.7333310255385408 0.6160072556131554 0.5075524904947084
0.2847794849864040 0.4539314483419224 0.6368200183445778
0.2813140657300853 0.5287204144618098 0.3672824882923982
0.6037912595924373 0.3883571029508711 0.4804046739831315
0.5975436274723835 0.6028876349079716 0.4955313555229149
0.7290265245420025 0.3917494348415701 0.4926563680680546
0.4070021622265951 0.4808056989802471 0.6460018700564691
0.2232333624649945 0.4774715609351585 0.4953390274372164
0.7875017674467243 0.5015032264798970 0.5080833837914903
0.3657103527314851 0.5279644763133916 0.2518379080472581
0.4178068173421154 0.6004958222116200 0.2420760701830160
0.3367608986193437 0.6074945251748917 0.2916393701716826
0.6597450255844679 0.6821746823818172 0.5546402604919576
0.6748708192833169 0.6842946158140155 0.4364617246614794
0.7359233138758594 0.7170241570828982 0.5124529157537522
0.4821012626085739 0.5335049909129056 0.5214830898094996
0.5229661080033262 0.4883773297344455 0.4831551784576654
```

S9-dim

Comment

```
1.00000000000000000000
20.000000000000000000 0.000000000000000000 0.000000000000000000
0.00000000000000000000 20.000000000000000000 0.000000000000000000
0.00000000000000000000 0.000000000000000000 15.000000000000000000
```

```
C      O      H      N      F
14      4      8      2      6
```

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.4086870843110439 | 0.5131680929048986 | 0.5102071108581470 |
| 0.3785496656660168 | 0.4854704568418002 | 0.5850538176812731 |
| 0.3099485874930265 | 0.4732168638039612 | 0.5841948714428492 |
| 0.2732227690392565 | 0.4890487786285010 | 0.5081027313852371 |
| 0.3034909615066692 | 0.5170774311857720 | 0.4326805367340614 |
| 0.3721148915512537 | 0.5296294688537967 | 0.4339690620453194 |
| 0.5921828756151677 | 0.4943484843784444 | 0.4893972849990751 |
| 0.6287607002629758 | 0.4347707817362365 | 0.4877628573971631 |
| 0.6231273730846280 | 0.5571601045900494 | 0.4970868258017684 |
| 0.6980468458389545 | 0.4383719332246951 | 0.4939686416081283 |
| 0.6926094191085833 | 0.5583506910303702 | 0.5039669210142872 |
| 0.7306054538112118 | 0.4997779289176904 | 0.5014383655217400 |
| 0.3882201088618905 | 0.5756098375175355 | 0.2852730924427457 |
| 0.7072780861948708 | 0.6794025374026563 | 0.5025159796296759 |
| 0.4956057316316828 | 0.5852201927179550 | 0.5523489271336762 |
| 0.4972856068102560 | 0.4334574437061838 | 0.4436963015636600 |
| 0.4108681850527584 | 0.5600370302187251 | 0.3681955794367576 |
| 0.7302500775614350 | 0.6164756208012074 | 0.5186042255465877 |
| 0.2856998903278502 | 0.4514703744251144 | 0.6426000663812382 |
| 0.2733308146302795 | 0.5293093778631713 | 0.3748847216903739 |
| 0.6024627690493046 | 0.3873360994542074 | 0.4818012085524444 |
| 0.5933584537665754 | 0.6023204572300020 | 0.4995206386248712 |
| 0.7271747160385811 | 0.3923825042328932 | 0.4918679012983832 |
| 0.4093258813036033 | 0.4748090131980736 | 0.6432547806403008 |
| 0.2194554491290701 | 0.4804260396355596 | 0.5076806360673674 |
| 0.7848191441573381 | 0.5023862592318121 | 0.5069158096691980 |
| 0.4787108829228318 | 0.5308686228253946 | 0.5150226731697588 |
| 0.5209316065470513 | 0.4857937807141376 | 0.4801377041708280 |
| 0.3860279149584424 | 0.5214417324979479 | 0.2306266703235611 |
| 0.4315600958550646 | 0.6200697664915086 | 0.2502973518053935 |
| 0.3261337994521543 | 0.6037853402973309 | 0.2853016312034103 |
| 0.6508383507903879 | 0.6952199199350616 | 0.5487855319525216 |
| 0.6940833673973710 | 0.6899031003267989 | 0.4145304033363856 |
| 0.7558124172724096 | 0.7222340171805206 | 0.5281092468717941 |

Geometries of **C1** used for functional testing

C1 XRD

Comment

1.0

| | | |
|---------------|---------------|--------------|
| 6.3853001595 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 11.2798004150 | 0.0000000000 |
| -0.1410626233 | 0.0000000000 | 3.6955086907 |

| O | N | C | H |
|---|---|----|---|
| 4 | 4 | 12 | 8 |

Direct

| | | |
|-------------|-------------|-------------|
| 0.511200011 | 0.624800026 | 0.261000007 |
| 0.488799989 | 0.375199974 | 0.738999963 |
| 0.988799989 | 0.124800026 | 0.238999993 |
| 0.011200011 | 0.875199974 | 0.761000037 |
| 0.569620013 | 0.534600019 | 0.078699999 |
| 0.430379987 | 0.465399981 | 0.921299994 |
| 0.930379987 | 0.034600019 | 0.421299994 |

| | | |
|-------------|-------------|-------------|
| 0.069620013 | 0.965399981 | 0.578700006 |
| 0.906499982 | 0.608810008 | 0.907999992 |
| 0.093500018 | 0.391189992 | 0.092000008 |
| 0.593500018 | 0.108810008 | 0.592000008 |
| 0.406499982 | 0.891189992 | 0.407999992 |
| 0.787580013 | 0.512950003 | 0.028600000 |
| 0.212419987 | 0.487049997 | 0.971400023 |
| 0.712419987 | 0.012950003 | 0.471399993 |
| 0.287580013 | 0.987049997 | 0.528599977 |
| 0.879800022 | 0.405800015 | 0.123899996 |
| 0.120199978 | 0.594200015 | 0.876100004 |
| 0.620199978 | 0.905799985 | 0.376100004 |
| 0.379800022 | 0.094199985 | 0.623899996 |
| 0.842999995 | 0.681240022 | 0.854799986 |
| 0.157000005 | 0.318759978 | 0.145200014 |
| 0.657000005 | 0.181240022 | 0.645200014 |
| 0.342999995 | 0.818759978 | 0.354799986 |
| 0.798500001 | 0.344090015 | 0.208800003 |
| 0.201499999 | 0.655910015 | 0.791199982 |
| 0.701499999 | 0.844089985 | 0.291199982 |
| 0.298500001 | 0.155909985 | 0.708800018 |

C1 PBE-revD3BJ

Comment

1.0

| | | |
|---------------|---------------|--------------|
| 6.4056577682 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 11.3354167938 | 0.0000000000 |
| -0.1800132925 | 0.0000000000 | 3.5986534546 |

| O | N | C | H |
|---|---|----|---|
| 4 | 4 | 12 | 8 |

Direct

| | | |
|-------------|-------------|-------------|
| 0.518603027 | 0.628238022 | 0.254808992 |
| 0.481397003 | 0.371762007 | 0.745190978 |
| 0.981396973 | 0.128238007 | 0.245190993 |
| 0.018603001 | 0.871761978 | 0.754809022 |
| 0.570614994 | 0.537275016 | 0.075562999 |
| 0.429385006 | 0.462725013 | 0.924436986 |
| 0.929385006 | 0.037275001 | 0.424436986 |
| 0.070615001 | 0.962724984 | 0.575563014 |
| 0.907953024 | 0.608883023 | 0.908721030 |
| 0.092046998 | 0.391117007 | 0.091279000 |
| 0.592046976 | 0.108883001 | 0.591278970 |
| 0.407952994 | 0.891116977 | 0.408721000 |
| 0.789108992 | 0.514110029 | 0.025665000 |
| 0.210890993 | 0.485890001 | 0.974335015 |
| 0.710891008 | 0.014110000 | 0.474335015 |
| 0.289108992 | 0.985889971 | 0.525664985 |
| 0.878084004 | 0.405173987 | 0.118404999 |
| 0.121916004 | 0.594825983 | 0.881595016 |
| 0.621915996 | 0.905174017 | 0.381594986 |
| 0.378084004 | 0.094825998 | 0.618404984 |
| 0.833613992 | 0.692403018 | 0.835561991 |
| 0.166385993 | 0.307597011 | 0.164437994 |
| 0.666386008 | 0.192403004 | 0.664438009 |

| | | |
|-------------|-------------|-------------|
| 0.333613992 | 0.807596982 | 0.335561991 |
| 0.783954978 | 0.332726985 | 0.214013994 |
| 0.216045007 | 0.667272985 | 0.785986006 |
| 0.716045022 | 0.832727015 | 0.285986006 |
| 0.283955008 | 0.167273000 | 0.714013994 |

C1 PBE-D3BJ

Comment

1.0

| | | |
|---------------|---------------|--------------|
| 6.4082860947 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 11.3385705948 | 0.0000000000 |
| -0.1664874386 | 0.0000000000 | 3.6197203419 |

| O | N | C | H |
|---|---|----|---|
| 4 | 4 | 12 | 8 |

Direct

| | | |
|-------------|-------------|-------------|
| 0.518148005 | 0.627662003 | 0.255964011 |
| 0.481851995 | 0.372337997 | 0.744036019 |
| 0.981851995 | 0.127662003 | 0.244036004 |
| 0.018147999 | 0.872337997 | 0.755963981 |
| 0.570442021 | 0.537090003 | 0.075935997 |
| 0.429556996 | 0.462909997 | 0.924063981 |
| 0.929557979 | 0.037090000 | 0.424064010 |
| 0.070442997 | 0.962909997 | 0.575936019 |
| 0.907954991 | 0.608812988 | 0.909148991 |
| 0.092045002 | 0.391187012 | 0.090851001 |
| 0.592045009 | 0.108813003 | 0.590851009 |
| 0.407954991 | 0.891187012 | 0.409148991 |
| 0.789040983 | 0.514033973 | 0.025676001 |
| 0.210959002 | 0.485965997 | 0.974323988 |
| 0.710959017 | 0.014034000 | 0.474323988 |
| 0.289041013 | 0.985966027 | 0.525676012 |
| 0.878089011 | 0.405191004 | 0.117896996 |
| 0.121910997 | 0.594808996 | 0.882103026 |
| 0.621910989 | 0.905191004 | 0.382102996 |
| 0.378089011 | 0.094809003 | 0.617896974 |
| 0.833977997 | 0.692364991 | 0.836157978 |
| 0.166022003 | 0.307635009 | 0.163841993 |
| 0.666022003 | 0.192365006 | 0.663842022 |
| 0.333977997 | 0.807635009 | 0.336158007 |
| 0.783976972 | 0.332760990 | 0.213469997 |
| 0.216022998 | 0.667239010 | 0.786530018 |
| 0.716023028 | 0.832760990 | 0.286529988 |
| 0.283977002 | 0.167238995 | 0.713469982 |

C1 PBE-dDsC

Comment

1.0

| | | |
|---------------|---------------|--------------|
| 6.3789539337 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 11.3051624298 | 0.0000000000 |
| -0.1731321132 | 0.0000000000 | 3.5489955023 |

| O | N | C | H |
|---|---|----|---|
| 4 | 4 | 12 | 8 |

Direct

| | | |
|-------------|-------------|-------------|
| 0.517508984 | 0.627135992 | 0.264407009 |
|-------------|-------------|-------------|

| | | |
|-------------|-------------|-------------|
| 0.482490987 | 0.372864008 | 0.735593021 |
| 0.982491016 | 0.127136007 | 0.235593006 |
| 0.017509000 | 0.872864008 | 0.764406979 |
| 0.570308983 | 0.537015975 | 0.078318000 |
| 0.429690987 | 0.462983996 | 0.921682000 |
| 0.929691017 | 0.037016001 | 0.421682000 |
| 0.070308998 | 0.962984025 | 0.578318000 |
| 0.907976985 | 0.609230995 | 0.909304976 |
| 0.092023000 | 0.390769005 | 0.090695001 |
| 0.592023015 | 0.109231003 | 0.590695024 |
| 0.407977015 | 0.890769005 | 0.409305006 |
| 0.789089978 | 0.514272988 | 0.027503001 |
| 0.210910007 | 0.485727012 | 0.972496986 |
| 0.710910022 | 0.014273000 | 0.472496986 |
| 0.289090008 | 0.985727012 | 0.527503014 |
| 0.877430022 | 0.404886007 | 0.119358003 |
| 0.122570001 | 0.595113993 | 0.880641997 |
| 0.622569978 | 0.904886007 | 0.380641997 |
| 0.377429992 | 0.095114000 | 0.619358003 |
| 0.832710981 | 0.692722023 | 0.835623980 |
| 0.167289004 | 0.307278007 | 0.164376006 |
| 0.667289019 | 0.192721993 | 0.664376020 |
| 0.332711011 | 0.807277977 | 0.335624009 |
| 0.782384992 | 0.332453012 | 0.216921002 |
| 0.217614993 | 0.667546988 | 0.783079028 |
| 0.717615008 | 0.832453012 | 0.283078998 |
| 0.282384992 | 0.167547002 | 0.716920972 |

C1 PBE-MBD

Comment

1.0

| | | |
|---------------|---------------|--------------|
| 6.4086909294 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 11.3202486038 | 0.0000000000 |
| -0.1782016874 | 0.0000000000 | 3.6479150640 |

| O | N | C | H |
|---|---|----|---|
| 4 | 4 | 12 | 8 |

Direct

| | | |
|-------------|-------------|-------------|
| 0.518899977 | 0.628215015 | 0.252420992 |
| 0.481099993 | 0.371785015 | 0.747578979 |
| 0.981100023 | 0.128215000 | 0.247578993 |
| 0.018900000 | 0.871784985 | 0.752421021 |
| 0.570629001 | 0.537263989 | 0.074493997 |
| 0.429370999 | 0.462736011 | 0.925505996 |
| 0.929370999 | 0.037264001 | 0.425505996 |
| 0.070629001 | 0.962736011 | 0.574494004 |
| 0.907854021 | 0.608856976 | 0.908722997 |
| 0.092146002 | 0.391142994 | 0.091277003 |
| 0.592145979 | 0.108856998 | 0.591277003 |
| 0.407853991 | 0.891143024 | 0.408722997 |
| 0.789045990 | 0.514052987 | 0.025175000 |
| 0.210953996 | 0.485947013 | 0.974825025 |
| 0.710954010 | 0.014053000 | 0.474824995 |
| 0.289045990 | 0.985947013 | 0.525174975 |
| 0.878275990 | 0.405155987 | 0.118098997 |

| | | |
|-------------|-------------|-------------|
| 0.121724002 | 0.594843984 | 0.881901026 |
| 0.621724010 | 0.905156016 | 0.381900996 |
| 0.378275990 | 0.094843999 | 0.618098974 |
| 0.833589017 | 0.692502975 | 0.835402012 |
| 0.166410998 | 0.307496995 | 0.164598003 |
| 0.666410983 | 0.192503005 | 0.664597988 |
| 0.333588988 | 0.807497025 | 0.335402012 |
| 0.784434974 | 0.332545012 | 0.213652998 |
| 0.215564996 | 0.667455018 | 0.786346972 |
| 0.715565026 | 0.832544982 | 0.286347002 |
| 0.284435004 | 0.167455003 | 0.713653028 |

C1 PBE-RP

Comment

1.0

| | | |
|---------------|---------------|--------------|
| 6.4153819084 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 11.4782838821 | 0.0000000000 |
| -0.2165948994 | 0.0000000000 | 3.6097606126 |

| O | N | C | H |
|---|---|----|---|
| 4 | 4 | 12 | 8 |

Direct

| | | |
|-------------|-------------|-------------|
| 0.519770026 | 0.628165007 | 0.248694003 |
| 0.480230004 | 0.371834993 | 0.751305997 |
| 0.980229974 | 0.128165007 | 0.251305997 |
| 0.019770000 | 0.871834993 | 0.748694003 |
| 0.571071982 | 0.537202001 | 0.074262001 |
| 0.428927988 | 0.462797999 | 0.925737977 |
| 0.928928018 | 0.037202001 | 0.425738007 |
| 0.071071997 | 0.962797999 | 0.574262023 |
| 0.907687008 | 0.607814014 | 0.910522997 |
| 0.092312999 | 0.392185986 | 0.089477003 |
| 0.592312992 | 0.107813999 | 0.589477003 |
| 0.407687008 | 0.892185986 | 0.410522997 |
| 0.789315999 | 0.513939977 | 0.025366001 |
| 0.210684001 | 0.486059994 | 0.974633992 |
| 0.710684001 | 0.013940000 | 0.474633992 |
| 0.289315999 | 0.986060023 | 0.525366008 |
| 0.878449023 | 0.406069010 | 0.116527997 |
| 0.121551000 | 0.593931019 | 0.883472025 |
| 0.621550977 | 0.906068981 | 0.383471996 |
| 0.378448993 | 0.093930997 | 0.616527975 |
| 0.832746029 | 0.690061986 | 0.839044988 |
| 0.167254001 | 0.309938014 | 0.160955995 |
| 0.667253971 | 0.190062001 | 0.660955012 |
| 0.332745999 | 0.809938014 | 0.339044005 |
| 0.784886003 | 0.334643990 | 0.210467994 |
| 0.215113997 | 0.665355980 | 0.789532006 |
| 0.715113997 | 0.834644020 | 0.289532006 |
| 0.284886003 | 0.165355995 | 0.710467994 |

C1 PBEsol

Comment

1.0

| | | |
|--------------|--------------|--------------|
| 6.3748950958 | 0.0000000000 | 0.0000000000 |
|--------------|--------------|--------------|

| | | | |
|---|---------------|---------------|--------------|
| | 0.0000000000 | 11.1258277893 | 0.0000000000 |
| | -0.1812287901 | 0.0000000000 | 3.5172462170 |
| O | N | C | H |
| 4 | 4 | 12 | 8 |

Direct

| | | |
|-------------|-------------|-------------|
| 0.518629014 | 0.630321026 | 0.257806003 |
| 0.481370986 | 0.369679004 | 0.742193997 |
| 0.981370986 | 0.130320996 | 0.242193997 |
| 0.018629000 | 0.869678974 | 0.757806003 |
| 0.570583999 | 0.537966013 | 0.075943999 |
| 0.429416001 | 0.462033987 | 0.924055994 |
| 0.929416001 | 0.037966002 | 0.424055994 |
| 0.070583999 | 0.962033987 | 0.575944006 |
| 0.908070982 | 0.611042976 | 0.908523977 |
| 0.091929004 | 0.388956994 | 0.091476001 |
| 0.591929018 | 0.111042999 | 0.591476023 |
| 0.408071011 | 0.888957024 | 0.408524007 |
| 0.788668990 | 0.514367998 | 0.024860000 |
| 0.211330995 | 0.485632002 | 0.975139976 |
| 0.711331010 | 0.014368000 | 0.475140005 |
| 0.288668990 | 0.985632002 | 0.524860024 |
| 0.877300978 | 0.403216004 | 0.117688000 |
| 0.122699000 | 0.596783996 | 0.882312000 |
| 0.622699022 | 0.903216004 | 0.382312000 |
| 0.377301008 | 0.096784003 | 0.617688000 |
| 0.833422005 | 0.696720004 | 0.833657980 |
| 0.166577995 | 0.303279996 | 0.166342005 |
| 0.666577995 | 0.196720004 | 0.666342020 |
| 0.333422005 | 0.803279996 | 0.333658010 |
| 0.782085001 | 0.328862011 | 0.214036003 |
| 0.217914999 | 0.671137989 | 0.785964012 |
| 0.717914999 | 0.828862011 | 0.285964012 |
| 0.282085001 | 0.171138003 | 0.714035988 |

C1 PBE-TS

Comment

1.0

| | | | |
|---|---------------|---------------|--------------|
| | 6.4075899124 | 0.0000000000 | 0.0000000000 |
| | 0.0000000000 | 11.4355010986 | 0.0000000000 |
| | -0.1544021020 | 0.0000000000 | 3.6597394844 |
| O | N | C | H |
| 4 | 4 | 12 | 8 |

Direct

| | | |
|-------------|-------------|-------------|
| 0.517235994 | 0.627303004 | 0.249626994 |
| 0.482764006 | 0.372696996 | 0.750373006 |
| 0.982764006 | 0.127303004 | 0.250373006 |
| 0.017236000 | 0.872696996 | 0.749626994 |
| 0.570308983 | 0.536862016 | 0.075101003 |
| 0.429690987 | 0.463138014 | 0.924898982 |
| 0.929691017 | 0.036862001 | 0.424899012 |
| 0.070308998 | 0.963137984 | 0.575101018 |
| 0.908069015 | 0.607882977 | 0.911065996 |
| 0.091931000 | 0.392116994 | 0.088933997 |
| 0.591930985 | 0.107882999 | 0.588934004 |

| | | |
|-------------|-------------|-------------|
| 0.408069015 | 0.892117023 | 0.411065996 |
| 0.789102018 | 0.513804018 | 0.026055999 |
| 0.210897997 | 0.486196011 | 0.973944008 |
| 0.710897982 | 0.013804000 | 0.473944008 |
| 0.289101988 | 0.986195982 | 0.526055992 |
| 0.877970994 | 0.405815989 | 0.116131000 |
| 0.122028999 | 0.594183981 | 0.883868992 |
| 0.622029006 | 0.905816019 | 0.383868992 |
| 0.377970994 | 0.094183996 | 0.616131008 |
| 0.833387971 | 0.690553010 | 0.840059996 |
| 0.166611999 | 0.309446990 | 0.159940004 |
| 0.666612029 | 0.190552995 | 0.659940004 |
| 0.333388001 | 0.809446990 | 0.340059996 |
| 0.783329010 | 0.334120005 | 0.210598007 |
| 0.216671005 | 0.665880024 | 0.789402008 |
| 0.716670990 | 0.834119976 | 0.289402008 |
| 0.283329010 | 0.165879995 | 0.710597992 |

C1 vdW-DF2

Comment

1.0

| | | |
|---------------|---------------|--------------|
| 6.4070591927 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 11.2976064682 | 0.0000000000 |
| -0.1904672490 | 0.0000000000 | 3.5445682152 |

| O | N | C | H |
|---|---|----|---|
| 4 | 4 | 12 | 8 |

Direct

| | | |
|-------------|-------------|-------------|
| 0.519098997 | 0.628221989 | 0.261869013 |
| 0.480901003 | 0.371778011 | 0.738130987 |
| 0.980901003 | 0.128222004 | 0.238131002 |
| 0.019099001 | 0.871778011 | 0.761869013 |
| 0.570890009 | 0.537104011 | 0.077583000 |
| 0.429109991 | 0.462895989 | 0.922416985 |
| 0.929109991 | 0.037103999 | 0.422417015 |
| 0.070890002 | 0.962895989 | 0.577583015 |
| 0.907573998 | 0.609531999 | 0.908611000 |
| 0.092426002 | 0.390468001 | 0.091389000 |
| 0.592426002 | 0.109531999 | 0.591389000 |
| 0.407573998 | 0.890468001 | 0.408611000 |
| 0.789355993 | 0.513984978 | 0.026249999 |
| 0.210644007 | 0.486014992 | 0.973749995 |
| 0.710644007 | 0.013985000 | 0.473749995 |
| 0.289355993 | 0.986015022 | 0.526250005 |
| 0.878287971 | 0.404399008 | 0.119243003 |
| 0.121711999 | 0.595601022 | 0.880756974 |
| 0.621712029 | 0.904398978 | 0.380757004 |
| 0.378288001 | 0.095601000 | 0.619243026 |
| 0.832158029 | 0.693448007 | 0.834437013 |
| 0.167842001 | 0.306551993 | 0.165563002 |
| 0.667841971 | 0.193448007 | 0.665562987 |
| 0.332157999 | 0.806551993 | 0.334437013 |
| 0.783860981 | 0.331465006 | 0.216206998 |
| 0.216139004 | 0.668534994 | 0.783792973 |
| 0.716139019 | 0.831465006 | 0.283793002 |

0.283861011

0.168534994

0.716207027

C1 vdW-DF2-B86R

Comment

1.0

| | | |
|---------------|---------------|--------------|
| 6.4027280807 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 11.3245315552 | 0.0000000000 |
| -0.1695174090 | 0.0000000000 | 3.5607640980 |

| O | N | C | H |
|---|---|----|---|
| 4 | 4 | 12 | 8 |

Direct

| | | |
|-------------|-------------|-------------|
| 0.518016994 | 0.627071977 | 0.264683008 |
| 0.481983006 | 0.372927994 | 0.735316992 |
| 0.981983006 | 0.127072006 | 0.235317007 |
| 0.018017000 | 0.872928023 | 0.764683008 |
| 0.570577979 | 0.536813974 | 0.078305997 |
| 0.429421991 | 0.463185996 | 0.921693981 |
| 0.929422021 | 0.036814000 | 0.421694010 |
| 0.070578001 | 0.963186026 | 0.578306019 |
| 0.907860994 | 0.609247029 | 0.909763992 |
| 0.092138998 | 0.390753001 | 0.090236001 |
| 0.592139006 | 0.109246999 | 0.590236008 |
| 0.407860994 | 0.890752971 | 0.409763992 |
| 0.789315999 | 0.513998985 | 0.026907001 |
| 0.210684001 | 0.486001015 | 0.973092973 |
| 0.710684001 | 0.013999000 | 0.473093003 |
| 0.289315999 | 0.986001015 | 0.526907027 |
| 0.877961993 | 0.404715002 | 0.118894003 |
| 0.122037999 | 0.595284998 | 0.881106019 |
| 0.622038007 | 0.904715002 | 0.381105989 |
| 0.377961993 | 0.095284998 | 0.618893981 |
| 0.832717001 | 0.693014979 | 0.836358011 |
| 0.167282999 | 0.306984991 | 0.163642004 |
| 0.667282999 | 0.193014994 | 0.663641989 |
| 0.332717001 | 0.806985021 | 0.336358011 |
| 0.782878995 | 0.332118005 | 0.215551004 |
| 0.217121005 | 0.667882025 | 0.784448981 |
| 0.717121005 | 0.832117975 | 0.284449011 |
| 0.282878995 | 0.167881995 | 0.715551019 |

C1 SCAN-rVV10

Comment

1.0

| | | |
|---------------|---------------|--------------|
| 6.3201589584 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 10.7764949799 | 0.0000000000 |
| -0.2276977966 | 0.0000000000 | 3.2130110246 |

| O | N | C | H |
|---|---|----|---|
| 4 | 4 | 12 | 8 |

Direct

| | | |
|-------------|-------------|-------------|
| 0.519111991 | 0.635583997 | 0.271097988 |
| 0.480888009 | 0.364416003 | 0.728901982 |
| 0.980888009 | 0.135583997 | 0.228901997 |
| 0.019112000 | 0.864416003 | 0.771098018 |
| 0.571193993 | 0.538268030 | 0.083144002 |

| | | |
|-------------|-------------|-------------|
| 0.428806007 | 0.461732000 | 0.916855991 |
| 0.928806007 | 0.038268000 | 0.416855991 |
| 0.071194001 | 0.961731970 | 0.583144009 |
| 0.905952990 | 0.614688993 | 0.907028019 |
| 0.094047002 | 0.385311007 | 0.092972003 |
| 0.594047010 | 0.114689000 | 0.592971981 |
| 0.405952990 | 0.885311007 | 0.407027990 |
| 0.789847016 | 0.514178991 | 0.031104000 |
| 0.210152999 | 0.485821009 | 0.968895972 |
| 0.710152984 | 0.014179000 | 0.468896002 |
| 0.289846987 | 0.985821009 | 0.531104028 |
| 0.879042029 | 0.399378002 | 0.125860006 |
| 0.120958000 | 0.600621998 | 0.874140024 |
| 0.620957971 | 0.899378002 | 0.374139994 |
| 0.379042000 | 0.100621998 | 0.625859976 |
| 0.828054011 | 0.701605022 | 0.828230977 |
| 0.171946004 | 0.298395008 | 0.171768993 |
| 0.671945989 | 0.201605007 | 0.671769023 |
| 0.328054011 | 0.798394978 | 0.328231007 |
| 0.784590006 | 0.323500007 | 0.229387999 |
| 0.215409994 | 0.676500022 | 0.770612001 |
| 0.715409994 | 0.823499978 | 0.270612001 |
| 0.284590006 | 0.176499993 | 0.729387999 |

C1 TPSS

Comment

1.0

| | | |
|---------------|---------------|--------------|
| 6.4253492355 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 11.9709177017 | 0.0000000000 |
| -0.1419023773 | 0.0000000000 | 4.1707267453 |

| O | N | C | H |
|---|---|----|---|
| 4 | 4 | 12 | 8 |

Direct

| | | |
|-------------|-------------|-------------|
| 0.516349971 | 0.623592019 | 0.211266994 |
| 0.483649999 | 0.376408011 | 0.788733006 |
| 0.983650029 | 0.123591997 | 0.288733006 |
| 0.016349999 | 0.876407981 | 0.711266994 |
| 0.569868028 | 0.535835028 | 0.062788002 |
| 0.430132002 | 0.464165002 | 0.937211990 |
| 0.930131972 | 0.035835002 | 0.437211990 |
| 0.069867998 | 0.964164972 | 0.562788010 |
| 0.908973992 | 0.602832019 | 0.918528020 |
| 0.091026001 | 0.397168010 | 0.081472002 |
| 0.591026008 | 0.102831997 | 0.581471980 |
| 0.408973992 | 0.897167981 | 0.418527991 |
| 0.789355993 | 0.513482988 | 0.021590000 |
| 0.210644007 | 0.486517012 | 0.978410006 |
| 0.710644007 | 0.013483000 | 0.478410006 |
| 0.289355993 | 0.986517012 | 0.521589994 |
| 0.877404988 | 0.410670996 | 0.104737997 |
| 0.122594997 | 0.589329004 | 0.895262003 |
| 0.622595012 | 0.910670996 | 0.395262003 |
| 0.377404988 | 0.089328997 | 0.604737997 |
| 0.835781991 | 0.681590974 | 0.855206013 |

| | | |
|-------------|-------------|-------------|
| 0.164217994 | 0.318408996 | 0.144794002 |
| 0.664218009 | 0.181591004 | 0.644793987 |
| 0.335781991 | 0.818409026 | 0.355206013 |
| 0.782966018 | 0.342667997 | 0.188598007 |
| 0.217033997 | 0.657332003 | 0.811402023 |
| 0.717033982 | 0.842667997 | 0.311401993 |
| 0.282965988 | 0.157332003 | 0.688597977 |

C1 TPSS-D3BJ

Comment

1.0

| | | |
|---------------|---------------|--------------|
| 6.4014611244 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 11.3429775238 | 0.0000000000 |
| -0.2078770924 | 0.0000000000 | 3.5403983372 |

| O | N | C | H |
|---|---|----|---|
| 4 | 4 | 12 | 8 |

Direct

| | | |
|-------------|-------------|-------------|
| 0.519752979 | 0.629791021 | 0.249731004 |
| 0.480246991 | 0.370209008 | 0.750268996 |
| 0.980247021 | 0.129791006 | 0.250268996 |
| 0.019753000 | 0.870208979 | 0.749731004 |
| 0.571056008 | 0.537388027 | 0.073912002 |
| 0.428943992 | 0.462612003 | 0.926087976 |
| 0.928943992 | 0.037388001 | 0.426088005 |
| 0.071056001 | 0.962611973 | 0.573912024 |
| 0.907922029 | 0.609112024 | 0.910807014 |
| 0.092078000 | 0.390888005 | 0.089193001 |
| 0.592077971 | 0.109112002 | 0.589192986 |
| 0.407922000 | 0.890887976 | 0.410807014 |
| 0.789710999 | 0.513965011 | 0.025304001 |
| 0.210289001 | 0.486034989 | 0.974695981 |
| 0.710289001 | 0.013965000 | 0.474696010 |
| 0.289710999 | 0.986034989 | 0.525304019 |
| 0.878289998 | 0.404790014 | 0.116327003 |
| 0.121710002 | 0.595210016 | 0.883673012 |
| 0.621710002 | 0.904789984 | 0.383673012 |
| 0.378289998 | 0.095210001 | 0.616326988 |
| 0.833368003 | 0.692234993 | 0.839419007 |
| 0.166631997 | 0.307765007 | 0.160580993 |
| 0.666631997 | 0.192234993 | 0.660580993 |
| 0.333368003 | 0.807765007 | 0.339419007 |
| 0.784785986 | 0.332536012 | 0.210049003 |
| 0.215213999 | 0.667464018 | 0.789951980 |
| 0.715214014 | 0.832535982 | 0.289950997 |
| 0.284785986 | 0.167464003 | 0.710048020 |

C1 TPSS-TS

Comment

1.0

| | | |
|---------------|---------------|--------------|
| 6.4014620781 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 11.3429746628 | 0.0000000000 |
| -0.2078768688 | 0.0000000000 | 3.5403945290 |

| O | N | C | H |
|---|---|----|---|
| 4 | 4 | 12 | 8 |

Direct

| | | |
|-------------|-------------|-------------|
| 0.519752979 | 0.629791021 | 0.249731004 |
| 0.480246991 | 0.370209008 | 0.750268996 |
| 0.980247021 | 0.129791006 | 0.250268996 |
| 0.019753000 | 0.870208979 | 0.749731004 |
| 0.571056008 | 0.537388027 | 0.073912002 |
| 0.428943992 | 0.462612003 | 0.926087976 |
| 0.928943992 | 0.037388001 | 0.426088005 |
| 0.071056001 | 0.962611973 | 0.573912024 |
| 0.907922029 | 0.609112024 | 0.910807014 |
| 0.092078000 | 0.390888005 | 0.089193001 |
| 0.592077971 | 0.109112002 | 0.589192986 |
| 0.407922000 | 0.890887976 | 0.410807014 |
| 0.789710999 | 0.513965011 | 0.025304001 |
| 0.210289001 | 0.486034989 | 0.974695981 |
| 0.710289001 | 0.013965000 | 0.474696010 |
| 0.289710999 | 0.986034989 | 0.525304019 |
| 0.878291011 | 0.404790014 | 0.116327003 |
| 0.121708997 | 0.595210016 | 0.883673012 |
| 0.621708989 | 0.904789984 | 0.383673012 |
| 0.378291011 | 0.095210001 | 0.616326988 |
| 0.833368003 | 0.692236006 | 0.839419007 |
| 0.166631997 | 0.307763994 | 0.160580993 |
| 0.666631997 | 0.192236006 | 0.660580993 |
| 0.333368003 | 0.807763994 | 0.339419007 |
| 0.784785986 | 0.332536012 | 0.210048005 |
| 0.215213999 | 0.667464018 | 0.789951980 |
| 0.715214014 | 0.832535982 | 0.289952010 |
| 0.284785986 | 0.167464003 | 0.710048020 |

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