Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information to the manuscript

Spin contamination as a major problem in the calculation of spin-spin coupling in triplet biradicals

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Contents

All cartesian coordinates are given in atomic units (bohr), total energies in Hartree (E_h), and zero field splitting parameters as well as magnetic anisotropies in cm^{-1}. Expectation values of the square of the spin operator (S^2) are given in atomic units ($h/2\pi$). For convenience we give the conversion factor to SI units:

1 bohr	=	$5.291772083535412 * 10^{-11}$	m
1 E_h	=	$2.625499617967463 * 10^{3}$	kJ mol^{-1}
1 cm^{-1}	=	$1.196265646149163 * 10^{-2}$	kJ mol^{-1}
$h/(2\pi)$	=	$1.054571628251774 * 10^{-34}$	J s

Computational Details

The geometries of the molecular structures were optimized using density functional theory with the B3LYP hybrid functional [1–4] and polaritzed valence triple zeta (TZVP) basis sets [5]. The density functional calculations were performed with a program developed in-house [6] and built upon the integral-direct TURBOMOLE engine [7, 8]. For the geometry relaxation steps the Berny algorithm [9] as implemented in the program GAUSSIAN03 [10] was used.

The spin-dipolar contribution to the magnetic anisotropy and zero field splitting tensor is a first-order property which can be expressed as a two-electron expectation value. This needs the two-particle spin density matrix which was originally derived by McWeeney and Mizuno [11] who showed that for one-determinant wave functions the two-particle spin density matrix can be constructed from the one-particle one. More specifically, the magnetic anisotropy tensor **M** is given by [12] ($\kappa,\lambda = x,y,z$)

$$M_{\kappa\lambda} = \frac{g_e^2}{2c^2} \sum_{\mu,\nu,\rho,\sigma} \Gamma^S_{\mu\nu,\rho\sigma} \int' \chi_\mu(\vec{r}_1)\chi_\rho(\vec{r}_2) \left(\frac{\delta_{\kappa\lambda}}{r_{12}^3} - \frac{3\kappa_{12}\lambda_{12}}{r_{12}^5} \right) \chi_\nu(\vec{r}_1)\chi_\sigma(\vec{r}_2)\,\mathrm{d}\vec{r}_1\,\mathrm{d}\vec{r}_2 \tag{1}$$

where the prime at the integral sign indicates that the singularity at $r_{12} = 0$ is excluded (this makes **M** traceless). In our calculations we used the g value of the free electron $g_e = 2.002319304362$. The two-particle spin density matrix is then expressed through the one-particle spin densities (this only holds for single Slater determinant wave functions [11])

$$\Gamma^S_{\mu\nu,\rho\sigma} = P^S_{\mu\nu} P^S_{\rho\sigma} - P^S_{\mu\sigma} P^S_{\rho\nu} \tag{2}$$

where $P^S_{\mu\nu} = P^\alpha_{\mu\nu} - P^\beta_{\mu\nu}$ are the elements of the difference of the alpha and beta density one-particle density matrices. The zero field splitting tensor can be easily obtained from the magnetic anisotropy

$$\mathbf{D} = \frac{1}{S\left(S - \frac{1}{2}\right)} \mathbf{M} \tag{3}$$

as explained in detail in Ref. [12]. For the triplets (*S*=1) investigated in this manuscript, $\mathbf{D} = 2\mathbf{M}$. For the doublets, the prefactor is undefined (division by zero) but $\mathbf{M} = 0$ if computed from a pure spin wave function. Note that even for doublets, a nonzero **M** may be obtained from a wave function that is spin contaminated (still, **D** is undefined).

A spin-restricted (high-spin) Kohn-Sham wave function is a Slater determinant built from a

set of doubly occupied orbitals, augmented by one or more singly occupied (spin-up) orbitals. In this case the one-particle spin density matrix only depends on the coefficients the singly occupied MOs ϕ_x

$$P^S_{\mu\nu} = \sum_x C^*_{\mu x} C_{\nu x} \,. \tag{4}$$

(the sum goes over the singly occupied orbitals only). This determinant is a pure spin function with $S = n/2$, n being the number of singly occupied orbitals. In the special case *n*=1, it is easy to see that all elements of the two-particle spin density matrix vanish (thus $\mathbf{M} = 0$):

$$\Gamma^S_{\mu\nu,\rho\sigma} = P^S_{\mu\nu} P^S_{\rho\sigma} - P^S_{\mu\sigma} P^S_{\rho\nu} = \left(C^*_{\mu x} C_{\nu x}\right)\left(C^*_{\rho x} C_{\sigma x}\right) - \left(C^*_{\mu x} C_{\sigma x}\right)\left(C^*_{\rho x} C_{\nu x}\right) = 0 \,. \tag{5}$$

The singly occupied orbitals used to calculate the spin density matrix need not come from a spin-restricted calculation: if one starts from a spin-unrestricted calculation with a given expectation value $\langle S_z \rangle = n/2$, then in most cases there are exactly *n* natural orbitals with occupation number close to unity, and one can take these to define a one-particle spin density according to Eq. (4), using then Eq. (2) to define the two-particle density matrix („quasi-restricted“ approach). In all cases investigated in this communication, the resulting magnetic anisotropy or ZFS tensors were very similar to those obtained from the self-consistent orbitals of a spin-restricted calculation.

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Triplet C_3H_6

Total energy: -117.845213 E_h S^2 expectation value: 2.0084

-2.36275238000000	0.52417711000000	-0.02949775000000	c
-2.30352089000000	2.56441970000000	-0.13468720000000	h
-4.19162372000000	-0.38894974000000	0.00662707000000	h
-0.00052611000000	-0.99773529000000	0.03252732000000	c
0.01016897000000	-2.37603100000000	-1.53726968000000	h
-0.01438364000000	-2.24341424000000	1.71922644000000	h
2.36231332000000	0.52176394000000	-0.02101407000000	c
2.32552957000000	2.53752738000000	0.31717951000000	h
4.17962072000000	-0.38278665000000	-0.26316917000000	h

Spin-dipolar contribution to ZFS tensor (cm^{-1}) from spin-unrestricted calculation

	X	Y	Z
X	-0.0008262	0.0006673	-0.0052244
Y	0.0006673	0.0775311	0.0087652
Z	-0.0052244	0.0087652	-0.0767049

Spin-dipolar contribution to ZFS tensor (cm^{-1}) from quasi-restricted calculation

	X	Y	Z
X	-0.0590061	-0.0001831	0.0014548
Y	-0.0001831	0.0257439	0.0020890
Z	0.0014548	0.0020890	0.0332622

Triplet C_5H_{10}

Total energy: -196.499586 E_h S^2 expectation value: 2.0075

4.78482310000000	-0.60347357000000	0.01466073000000	c
6.53922485000000	0.15101551000000	-0.71558864000000	h
4.85685082000000	-2.39381122000000	1.00389450000000	h
2.42101573000000	0.91332566000000	-0.03115525000000	c
2.37562963000000	2.20004268000000	1.61085512000000	h
2.41699205000000	2.16179477000000	-1.68478425000000	h
-0.00014351000000	-0.68179145000000	-0.00270061000000	c
0.02167936000000	-1.92711453000000	1.64905695000000	h
-0.02115341000000	-1.91497001000000	-1.66345533000000	h
-2.42107700000000	0.91180729000000	0.03677614000000	c
-2.37781780000000	2.21146746000000	-1.59502647000000	h
-2.41731363000000	2.15011999000000	1.69886816000000	h
-4.78498443000000	-0.60453425000000	-0.01801612000000	c
-6.55328225000000	0.17396044000000	0.65129814000000	h
-4.83861295000000	-2.42450712000000	-0.95250750000000	h

Spin-dipolar contribution to ZFS tensor (cm^{-1}) from spin-unrestricted calculation

	X	Y	Z
X	0.0365390	-0.0010417	-0.0279393
Y	-0.0010417	0.0288804	-0.0011336
Z	-0.0279393	-0.0011336	-0.0654194

Spin-dipolar contribution to ZFS tensor (cm^{-1}) from quasi-restricted calculation

	X	Y	Z
X	-0.0138879	0.0000181	0.0003055
Y	0.0000181	0.0068111	0.0000031
Z	0.0003055	0.0000031	0.0070769

Triplet C_7H_{14}

Total energy: -275.153593 E_h S^2 expectation value: 2.0076

-2.41721596000000	-0.71286723000000	-0.00797194000000	c
-2.40252185000000	-1.97421083000000	-1.64847380000000	h
-2.45199262000000	-1.93635509000000	1.66264320000000	h
-0.00020239000000	0.87298893000000	0.01313429000000	c
0.00356414000000	2.13464982000000	-1.63052353000000	h
-0.00372617000000	2.10293285000000	1.68076590000000	h
2.41734942000000	-0.71210031000000	-0.00068937000000	c
2.44093458000000	-1.91591630000000	-1.68568152000000	h
2.41267191000000	-1.99323637000000	1.62457328000000	h
4.84009184000000	0.87763175000000	0.05637094000000	c
4.84059169000000	2.09081023000000	1.73796691000000	h
4.79503087000000	2.20600749000000	-1.55198891000000	h
7.20576403000000	-0.63508551000000	-0.02587254000000	c
8.98972227000000	0.16900096000000	0.56792564000000	h
7.24018863000000	-2.48073516000000	-0.90913401000000	h
-4.84009821000000	0.87814531000000	-0.06266467000000	c
-4.84374691000000	2.09000179000000	-1.74437313000000	h
-4.78935404000000	2.20556957000000	1.54647331000000	h
-7.20552306000000	-0.63441396000000	0.02770565000000	c
-8.98054030000000	0.14484708000000	-0.62292743000000	h
-7.25181617000000	-2.44915992000000	0.97267992000000	h

Spin-dipolar contribution to ZFS tensor (cm^{-1}) from spin-unrestricted calculation

	X	Y	Z
X	0.0477527	0.0008831	0.0244158
Y	0.0008831	0.0274458	-0.0015004
Z	0.0244158	-0.0015004	-0.0751986

Spin-dipolar contribution to ZFS tensor (cm^{-1}) from quasi-restricted calculation

	X	Y	Z
X	-0.0041999	-0.0000016	-0.0000130
Y	-0.0000016	0.0021024	-0.0000000
Z	-0.0000130	-0.0000000	0.0020975

Triplet C_9H_{18}

Total energy: -353.807582 E_h S^2 expectation value: 2.0076

9.62646610000000	-0.65404280000000	-0.01288276000000	c
7.26141711000000	0.85986424000000	0.06140260000000	c
7.27696348000000	2.26318691000000	-1.46407058000000	h
7.19810251000000	1.98600688000000	1.81675146000000	h
4.83806368000000	-0.72498010000000	-0.09237864000000	c
4.84569658000000	-2.11614027000000	1.44201914000000	h
4.85137456000000	-1.80906246000000	-1.85513569000000	h
2.41997007000000	0.85270033000000	0.05386484000000	c
2.41822666000000	2.24397044000000	-1.48150524000000	h
2.42107043000000	1.94372212000000	1.81544016000000	h
0.00005318000000	-0.72492671000000	-0.08846480000000	c
-0.00170946000000	-2.11142384000000	1.45096175000000	h
0.00195363000000	-1.82099799000000	-1.84634400000000	h
-2.41999415000000	0.85303633000000	0.04770275000000	c
-2.42067655000000	2.23423954000000	-1.49671982000000	h
-2.41893402000000	1.95557872000000	1.80209629000000	h
-4.83791484000000	-0.72620503000000	-0.08414273000000	c
-4.84948813000000	-2.09692901000000	1.46848530000000	h
-4.84737549000000	-1.83360932000000	-1.83234239000000	h
-7.26168017000000	0.86117501000000	0.04268171000000	c
-7.27884459000000	2.23580936000000	-1.50819536000000	h
-7.19615323000000	2.01838657000000	1.77770071000000	h
-9.62624824000000	-0.65466532000000	-0.00078970000000	c
11.40552918000000	0.19382543000000	-0.55843890000000	h
9.66666142000000	-2.56850137000000	0.70977681000000	h
-9.67285416000000	-2.54168814000000	0.79057348000000	h
-11.40033931000000	0.17189063000000	-0.59301280000000	h

Spin-dipolar contribution to ZFS tensor (cm^{-1}) from spin-unrestricted calculation

	X	Y	Z
X	0.0498512	0.0006935	0.0003867
Y	0.0006935	0.0346948	-0.0461382
Z	0.0003867	-0.0461382	-0.0845460

Spin-dipolar contribution to ZFS tensor (cm^{-1}) from quasi-restricted calculation

	X	Y	Z
X	-0.0017441	-0.0000007	0.0000011
Y	-0.0000007	0.0008772	-0.0000176
Z	0.0000011	-0.0000176	0.0008668

Triplet $C_{11}H_{22}$

Total energy: -432.461539 E_h S^2 expectation value: 2.0076

12.04702824000000	-0.66627598000000	-0.03470215000000	c
9.68243874000000	0.84910925000000	0.01999927000000	c
9.69694947000000	2.11474365000000	1.66130948000000	h
9.62248147000000	2.12413800000000	-1.63097367000000	h
7.25823720000000	-0.74130695000000	0.03003505000000	c
7.26701848000000	-1.98973267000000	-1.62259420000000	h
7.26898541000000	-1.97866250000000	1.68881913000000	h
4.84071921000000	0.84392586000000	0.02219182000000	c
4.84585031000000	2.08934338000000	-1.63386819000000	h
4.83548572000000	2.09064755000000	1.67705601000000	h
2.42068060000000	-0.73975976000000	0.01640842000000	c
2.41682899000000	-1.98617825000000	1.67139311000000	h
2.42574652000000	-1.98643031000000	-1.63817918000000	h
-0.00005932000000	0.84288202000000	0.00804852000000	c
0.00556995000000	2.09071439000000	-1.64606280000000	h
-0.00710573000000	2.08811543000000	1.66383471000000	h
-2.42046828000000	-0.74077543000000	-0.00268121000000	c
-2.42545525000000	-1.98828594000000	1.65134699000000	h
-2.41665399000000	-1.98561816000000	-1.65869165000000	h
-4.84032520000000	0.84314620000000	-0.00332368000000	c
-4.83029651000000	2.10122449000000	-1.64944163000000	h
-4.85059398000000	2.07696454000000	1.66145165000000	h
-7.25845717000000	-0.74152580000000	-0.03239531000000	c
-7.28057209000000	-1.99033654000000	1.61970188000000	h
-7.25618802000000	-1.97826480000000	-1.69161002000000	h
12.09164939000000	-2.50370111000000	-0.93490898000000	h
13.82522168000000	0.13522581000000	0.57970928000000	h
-9.68207894000000	0.84973029000000	-0.03928128000000	c
-9.62594278000000	2.13226968000000	1.60645171000000	h
-9.69328097000000	2.10552841000000	-1.68706059000000	h
-12.04642049000000	-0.66585795000000	0.01561976000000	c
-13.81397283000000	0.11556638000000	-0.65364506000000	h
-12.10949276000000	-2.47702195000000	0.96644682000000	h

Spin-dipolar contribution to ZFS tensor (cm^{-1}) from spin-unrestricted calculation

	X	Y	Z
X	0.0503630	0.0009087	0.0259902
Y	0.0009087	0.0253114	-0.0012168
Z	0.0259902	-0.0012168	-0.0756744

Spin-dipolar contribution to ZFS tensor (cm^{-1}) from quasi-restricted calculation

	X	Y	Z
X	-0.0008768	-0.0000004	-0.0000030
Y	-0.0000004	0.0004390	-0.0000001
Z	-0.0000030	-0.0000001	0.0004378

Triplet $C_{13}H_{26}$

Total energy: -511.115357 E_h S^2 expectation value: 2.0076

-14.46857776000000	0.67429023000000	-0.01361819000000	c
-12.10153045000000	-0.83923774000000	-0.01135184000000	c
-12.09460771000000	-2.12781669000000	1.61904089000000	h
-12.07036850000000	-2.10403514000000	-1.66707062000000	h
-9.67926107000000	0.74714755000000	0.00486325000000	c
-9.68618281000000	2.00417478000000	-1.64084561000000	h
-9.68917400000000	1.97558715000000	1.67113177000000	h
-7.26141735000000	-0.83727203000000	-0.00784715000000	c
-7.25739112000000	-2.06481261000000	-1.67715571000000	h
-7.26516840000000	-2.10244451000000	1.63307537000000	h
-4.84089940000000	0.74549691000000	0.01635754000000	c
-4.84527235000000	1.97238494000000	1.68580113000000	h
-4.83669493000000	2.01098138000000	-1.62407008000000	h
-2.42037370000000	-0.83766617000000	0.00462163000000	c
-2.41705491000000	-2.06724656000000	-1.66300342000000	h
-2.42394682000000	-2.10106654000000	1.64674714000000	h
0.00033270000000	0.74498888000000	0.02662303000000	c
-0.00243977000000	1.97194410000000	1.69615710000000	h
0.00309877000000	2.01066163000000	-1.61373639000000	h
2.42096357000000	-0.83789028000000	0.01285598000000	c
2.42288398000000	-2.06793129000000	-1.65445036000000	h
2.41908353000000	-2.10095029000000	1.65525836000000	h
4.84137531000000	0.74511038000000	0.03292245000000	c
4.84697062000000	1.96071985000000	1.71063763000000	h
4.83599196000000	2.02149809000000	-1.59904512000000	h
-14.43745905000000	2.69305874000000	-0.34268399000000	h
-16.29053099000000	-0.23035478000000	0.19943078000000	h
7.26162319000000	-0.83770058000000	-0.00248452000000	c
7.27459131000000	-2.09984187000000	1.64078958000000	h
7.24852581000000	-2.06822971000000	-1.66957817000000	h
9.67920030000000	0.74678246000000	-0.00421432000000	c
9.69701810000000	1.97518534000000	1.66259411000000	h
9.67783701000000	2.00384612000000	-1.64945655000000	h
12.10093508000000	-0.83888894000000	-0.03078164000000	c
12.08498652000000	-2.13777531000000	1.59567976000000	h
12.08018699000000	-2.09594522000000	-1.68884522000000	h
14.46824667000000	0.67374471000000	-0.01457617000000	c
14.42520078000000	2.71779782000000	0.04747894000000	h
16.29621344000000	-0.24282184000000	-0.05410170000000	h

Spin-dipolar contribution to ZFS tensor (cm^{-1}) from spin-unrestricted calculation

	X	Y	Z
X	0.0556675	-0.0006756	-0.0057907
Y	-0.0006756	0.0505947	-0.0084842
Z	-0.0057907	-0.0084842	-0.1062623

Spin-dipolar contribution to ZFS tensor (cm^{-1}) from quasi-restricted calculation

	X	Y	Z
X	-0.0004950	0.0000003	0.0000008
Y	0.0000003	0.0002482	-0.0000003
Z	0.0000008	-0.0000003	0.0002468

Triplet $C_{15}H_{30}$

Total energy: -589.769451 E_h S^2 expectation value: 2.0076

16.88944806000000	-0.68041697000000	-0.04974227000000	c
14.52428839000000	0.83389449000000	0.01629236000000	c
14.53866310000000	2.08595510000000	1.66969228000000	h
14.46646539000000	2.12606623000000	-1.62061575000000	h
12.10078374000000	-0.75548549000000	0.01722781000000	c
12.10813919000000	-1.99438315000000	-1.64255745000000	h
12.11226825000000	-2.00244844000000	1.66899126000000	h
9.68315412000000	0.82958641000000	0.02075044000000	c
9.68304198000000	2.07937635000000	-1.63198091000000	h
9.68358326000000	2.07258734000000	1.67851918000000	h
7.26246822000000	-0.75312923000000	0.01857846000000	c
7.26239415000000	-2.00228552000000	1.67140664000000	h
7.26236289000000	-1.99670511000000	-1.63857371000000	h
4.84219081000000	0.83048005000000	0.02121879000000	c
4.84437123000000	2.08280373000000	-1.62940085000000	h
4.84068738000000	2.07116059000000	1.68061543000000	h
2.42116348000000	-0.75187940000000	0.01245509000000	c
2.41915603000000	-2.00511650000000	1.66237677000000	h
2.42291314000000	-1.99178221000000	-1.64752482000000	h
0.00038764000000	0.83096109000000	0.01601597000000	c
0.00471537000000	2.08797328000000	-1.63104447000000	h
-0.00398329000000	2.06710495000000	1.67880179000000	h
-2.42041799000000	-0.75183065000000	-0.00095926000000	c
-2.42468704000000	-2.00974985000000	1.64542072000000	h
-2.41577243000000	-1.98703939000000	-1.66439795000000	h
16.90828779000000	-2.56546407000000	-0.84621988000000	h
18.68282303000000	0.14511309000000	0.48398993000000	h
-4.84165097000000	0.83038489000000	0.00312166000000	c
-4.84773889000000	2.06390953000000	1.66776144000000	h
-4.83645050000000	2.08991049000000	-1.64197223000000	h
-7.26200632000000	-0.75328240000000	-0.01803955000000	c
-7.26832964000000	-2.01215421000000	1.62745996000000	h
-7.25523110000000	-1.98700811000000	-1.68230583000000	h
-9.68295572000000	0.82926616000000	-0.01561495000000	c
-9.68986425000000	2.06477486000000	1.64770204000000	h
-9.67700365000000	2.08650286000000	-1.66250079000000	h
-12.10044530000000	-0.75635320000000	-0.03545774000000	c
-12.11742804000000	-2.00561584000000	1.61648868000000	h
-12.10401837000000	-1.99307233000000	-1.69448417000000	h
-14.52582804000000	0.83592374000000	-0.03710360000000	c
-14.46261813000000	2.11815633000000	1.60824572000000	h
-14.53916942000000	2.08838105000000	-1.68682185000000	h
-16.88962305000000	-0.68081895000000	0.02899662000000	c
-18.64658124000000	0.06239057000000	-0.70687106000000	h
-16.95673857000000	-2.46314485000000	1.03336085000000	h

Spin-dipolar contribution to ZFS tensor (cm^{-1}) from spin-unrestricted calculation

	X	Y	Z
X	0.0511322	0.0032203	0.0254913
Y	0.0032203	0.0257765	-0.0048796
Z	0.0254913	-0.0048796	-0.0769087

Spin-dipolar contribution to ZFS tensor (cm^{-1}) from quasi-restricted calculation

	X	Y	Z
X	-0.0003134	-0.0000004	-0.0000002
Y	-0.0000004	0.0001568	-0.0000001
Z	-0.0000002	-0.0000001	0.0001565

Doublet $C_{14}H_{30}B$ (left) -- first carbon of $C_{15}H_{30}$ substituted by boron --

Total energy: -576.531135 E_h S^2 expectation value: 0.7538

16.88944806000000	-0.68041697000000	-0.04974227000000	b
14.52428839000000	0.83389449000000	0.01629236000000	c
14.53866310000000	2.08595510000000	1.66969228000000	h
14.46646539000000	2.12606623000000	-1.62061575000000	h
12.10078374000000	-0.75548549000000	0.01722781000000	c
12.10813919000000	-1.99438315000000	-1.64255745000000	h
12.11226825000000	-2.00244844000000	1.66899126000000	h
9.68315412000000	0.82958641000000	0.02075044000000	c
9.68304198000000	2.07937635000000	-1.63198091000000	h
9.68358326000000	2.07258734000000	1.67851918000000	h
7.26246822000000	-0.75312923000000	0.01857846000000	c
7.26239415000000	-2.00228552000000	1.67140664000000	h
7.26236289000000	-1.99670511000000	-1.63857371000000	h
4.84219081000000	0.83048005000000	0.02121879000000	c
4.84437123000000	2.08280373000000	-1.62940085000000	h
4.84068738000000	2.07116059000000	1.68061543000000	h
2.42116348000000	-0.75187940000000	0.01245509000000	c
2.41915603000000	-2.00511650000000	1.66237677000000	h
2.42291314000000	-1.99178221000000	-1.64752482000000	h
0.00038764000000	0.83096109000000	0.01601597000000	c
0.00471537000000	2.08797328000000	-1.63104447000000	h
-0.00398329000000	2.06710495000000	1.67880179000000	h
-2.42041799000000	-0.75183065000000	-0.00095926000000	c
-2.42468704000000	-2.00974985000000	1.64542072000000	h
-2.41577243000000	-1.98703939000000	-1.66439795000000	h
16.90828779000000	-2.56546407000000	-0.84621988000000	h
18.68282303000000	0.14511309000000	0.48398993000000	h
-4.84165097000000	0.83038489000000	0.00312166000000	c
-4.84773889000000	2.06390953000000	1.66776144000000	h
-4.83645050000000	2.08991049000000	-1.64197223000000	h
-7.26200632000000	-0.75328240000000	-0.01803955000000	c
-7.26832964000000	-2.01215421000000	1.62745996000000	h
-7.25523110000000	-1.98700811000000	-1.68230583000000	h
-9.68295572000000	0.82926616000000	-0.01561495000000	c
-9.68986425000000	2.06477486000000	1.64770204000000	h
-9.67700365000000	2.08650286000000	-1.66250079000000	h
-12.10044530000000	-0.75635320000000	-0.03545774000000	c
-12.11742804000000	-2.00561584000000	1.61648868000000	h
-12.10401837000000	-1.99307233000000	-1.69448417000000	h
-14.52582804000000	0.83592374000000	-0.03710360000000	c
-14.46261813000000	2.11815633000000	1.60824572000000	h
-14.53916942000000	2.08838105000000	-1.68682185000000	h
-16.88962305000000	-0.68081895000000	0.02899662000000	c
-18.64658124000000	0.06239057000000	-0.70687106000000	h
-16.95673857000000	-2.46314485000000	1.03336085000000	h

Note: this geometry is not optimized. The coordinates are taken from the optimized geometry of triplet $C_{15}H_{30}$

Spin-dipolar contribution to magnetic anisotropy tensor (cm^{-1}) from spin-unrestricted calculation

	X	Y	Z
X	0.0124620	0.0055161	0.0072689
Y	0.0055161	0.0048338	-0.0148635
Z	0.0072689	-0.0148635	-0.0172958

Spin-dipolar contribution to magnetic anisotropy tensor (cm^{-1}) from quasi-restricted calculation

	X	Y	Z
X	0.0000000	0.0000000	0.0000000
Y	0.0000000	-0.0000000	0.0000000
Z	0.0000000	0.0000000	-0.0000000

Doublet $C_{14}H_{30}B$ (right) -- last carbon of $C_{15}H_{30}$ substituted by boron --

Total energy: -576.530813 E_h S^2 expectation value: 0.7538

16.88944806000000	-0.68041697000000	-0.04974227000000	c
14.52428839000000	0.83389449000000	0.01629236000000	c
14.53866310000000	2.08595510000000	1.66969228000000	h
14.46646539000000	2.12606623000000	-1.62061575000000	h
12.10078374000000	-0.75548549000000	0.01722781000000	c
12.10813919000000	-1.99438315000000	-1.64255745000000	h
12.11226825000000	-2.00244844000000	1.66899126000000	h
9.68315412000000	0.82958641000000	0.02075044000000	c
9.68304198000000	2.07937635000000	-1.63198091000000	h
9.68358326000000	2.07258734000000	1.67851918000000	h
7.26246822000000	-0.75312923000000	0.01857846000000	c
7.26239415000000	-2.00228552000000	1.67140664000000	h
7.26236289000000	-1.99670511000000	-1.63857371000000	h
4.84219081000000	0.83048005000000	0.02121879000000	c
4.84437123000000	2.08280373000000	-1.62940085000000	h
4.84068738000000	2.07116059000000	1.68061543000000	h
2.42116348000000	-0.75187940000000	0.01245509000000	c
2.41915603000000	-2.00511650000000	1.66237677000000	h
2.42291314000000	-1.99178221000000	-1.64752482000000	h
0.00038764000000	0.83096109000000	0.01601597000000	c
0.00471537000000	2.08797328000000	-1.63104447000000	h
-0.00398329000000	2.06710495000000	1.67880179000000	h
-2.42041799000000	-0.75183065000000	-0.00095926000000	c
-2.42468704000000	-2.00974985000000	1.64542072000000	h
-2.41577243000000	-1.98703939000000	-1.66439795000000	h
16.90828779000000	-2.56546407000000	-0.84621988000000	h
18.68282303000000	0.14511309000000	0.48398993000000	h
-4.84165097000000	0.83038489000000	0.00312166000000	c
-4.84773889000000	2.06390953000000	1.66776144000000	h
-4.83645050000000	2.08991049000000	-1.64197223000000	h
-7.26200632000000	-0.75328240000000	-0.01803955000000	c
-7.26832964000000	-2.01215421000000	1.62745996000000	h
-7.25523110000000	-1.98700811000000	-1.68230583000000	h
-9.68295572000000	0.82926616000000	-0.01561495000000	c
-9.68986425000000	2.06477486000000	1.64770204000000	h
-9.67700365000000	2.08650286000000	-1.66250079000000	h
-12.10044530000000	-0.75635320000000	-0.03545774000000	c
-12.11742804000000	-2.00561584000000	1.61648868000000	h
-12.10401837000000	-1.99307233000000	-1.69448417000000	h
-14.52582804000000	0.83592374000000	-0.03710360000000	c
-14.46261813000000	2.11815633000000	1.60824572000000	h
-14.53916942000000	2.08838105000000	-1.68682185000000	h
-16.88962305000000	-0.68081895000000	0.02899662000000	b
-18.64658124000000	0.06239057000000	-0.70687106000000	h
-16.95673857000000	-2.46314485000000	1.03336085000000	h

Note: this geometry is not optimized. The coordinates are taken from the optimized geometry of triplet $C_{15}H_{30}$

Spin-dipolar contribution to magnetic anisotropy tensor (cm^{-1}) from spin-unrestricted calculation

	X	Y	Z
X	0.0132613	-0.0039068	0.0054749
Y	-0.0039068	0.0079824	0.0124241
Z	0.0054749	0.0124241	-0.0212437

Spin-dipolar contribution to magnetic anisotropy tensor (cm^{-1}) from quasi-restricted calculation

	X	Y	Z
X	0.0000000	0.0000000	0.0000000
Y	0.0000000	-0.0000000	0.0000000
Z	0.0000000	0.0000000	-0.0000000