

Towards an Understanding of Magnetic Interactions within a Series of
Tetrathiafulvalene- π Conjugated-Verdazyl Diradical Cation Systems.
A Density Functional Theory Study.

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Pilkington.²

Table S1. Calculated overlap integral between the magnetically active orbitals in the
broken symmetry solution.

	Overlap
(1)	-0.181
(2)	-0.076
(3)	0.042
(4)	-0.020
(5)	0.173
(6)	0.077
(7)	0.195
(8)	-0.021
(9)	-0.055
(10)	-0.059

UB3LYP/6-31G(d,p) optimized geometries for diradicals (1)-(10), xyz coordinates in
Å.

(1) charge and multiplicity: 1,3
8 6.386469 -0.901862 0.000879
6 5.226972 -0.564899 0.000410
7 4.152252 -1.455778 -0.000279
7 4.792611 0.759855 0.000075
7 2.843760 -1.120640 -0.000368
7 3.507833 1.185865 -0.000142
6 2.611710 0.193212 -0.000243
6 1.197176 0.582383 -0.000093
6 0.725805 1.853126 -0.000109
16 -0.007601 -0.698586 -0.000305
16 -0.987889 2.078715 -0.000372
6 -1.386450 0.378912 -0.000051
6 -2.703096 -0.084711 0.000100
16 -3.102534 -1.787575 -0.000101
16 -4.088868 0.983299 0.000504
6 -4.829861 -1.555502 0.000045
6 -5.281154 -0.287980 0.000305
1 4.367357 -2.445310 -0.001011
1 5.504692 1.480002 0.000807
1 1.361804 2.730212 0.000004

1 -5.453081 -2.441814 -0.000069
1 -6.324052 0.005807 0.000412

(2) charge and multiplicity: 1,3
8 7.755743 -0.525624 -0.000158
6 6.548854 -0.440276 0.000056
7 5.684598 -1.531586 -0.000516
7 5.848762 0.763141 0.000881
7 4.333121 -1.485103 -0.000564
7 4.503076 0.912940 0.000847
6 3.822230 -0.247427 0.000098
6 2.366756 -0.184709 -0.000025
6 1.658233 0.966509 -0.000171
6 0.219566 1.065996 -0.000181
6 -0.470275 2.245533 -0.000130
16 -0.803220 -0.378694 -0.000234
16 -2.195191 2.206444 -0.000156
6 -2.334398 0.468548 -0.000134
6 -3.560446 -0.191810 -0.000008
16 -3.690416 -1.937488 0.000307
16 -5.097679 0.647892 -0.000130
6 -5.434453 -1.976602 0.000332
6 -6.077029 -0.795495 0.000165
1 6.103016 -2.453327 -0.001137
1 6.397023 1.614091 0.001228
1 1.885292 -1.159268 -0.000116
1 2.194760 1.911244 -0.000250
1 0.001673 3.221064 -0.000270
1 -5.911830 -2.949184 0.000489
1 -7.152892 -0.667426 0.000184

(3) charge and multiplicity: 1,3
8 -9.088958 -0.322266 -0.000033
6 -7.878687 -0.360835 -0.000364
7 -7.131034 -1.533893 -0.000339
7 -7.059757 0.763636 0.000068
7 -5.781415 -1.627346 -0.000283
7 -5.705331 0.776835 0.000152
6 -5.143390 -0.447496 -0.000083
6 -3.692574 -0.532006 -0.000070
6 -2.855084 0.538043 0.000190
6 -1.432940 0.397629 0.000144
6 -0.569341 1.453578 0.000241
6 0.862870 1.375261 0.000179
6 1.694040 2.465674 0.000129
16 1.707471 -0.182752 0.000160
16 3.397752 2.221829 0.000128
6 3.333541 0.478201 0.000076
6 4.469529 -0.319077 -0.000023
16 4.392461 -2.071011 0.000658

16 6.098940 0.332619 -0.000796
6 6.122019 -2.315231 0.000122
6 6.899342 -1.219718 -0.000477
1 -7.641770 -2.407710 -0.000349
1 -7.518278 1.665885 0.000368
1 -3.299751 -1.545073 -0.000280
1 -3.278524 1.539134 0.000415
1 1.342098 3.490562 0.000182
1 6.480855 -3.337349 0.000344
1 7.982660 -1.220402 -0.000819
1 -1.042634 -0.620237 -0.000006
1 -0.972161 2.463613 0.000438

(4) charge and multiplicity: 1,3

8 -10.426670 0.167929 -0.000034
6 -9.221494 0.290820 0.000043
7 -8.557626 1.512656 -0.000028
7 -8.326513 -0.773390 0.000032
7 -7.217593 1.700821 -0.000035
7 -6.974181 -0.692835 0.000030
6 -6.497540 0.567923 0.000009
6 -5.057747 0.753196 -0.000004
6 -4.145177 -0.257379 0.000016
6 -2.740024 -0.020791 0.000005
6 -1.794604 -1.014559 0.000026
6 -0.397332 -0.758764 0.000016
6 0.558572 -1.739587 0.000037
6 1.973200 -1.538426 0.000030
6 2.893402 -2.558250 0.000052
16 2.687035 0.086098 -0.000007
16 4.569133 -2.178005 0.000042
6 4.366356 -0.441948 0.000003
6 5.431240 0.439955 -0.000016
16 5.213041 2.183376 -0.000055
16 7.111850 -0.077555 -0.000004
6 6.919779 2.565561 -0.000063
6 7.782537 1.537526 -0.000040
1 -9.128090 2.348592 -0.000080
1 -8.720926 -1.705332 0.000024
1 -4.735111 1.790643 -0.000032
1 -4.500059 -1.284893 0.000043
1 2.625164 -3.608176 0.000077
1 7.194906 3.613217 -0.000086
1 8.862134 1.626174 -0.000042
1 -2.406167 1.016707 -0.000021
1 -2.122268 -2.052785 0.000052
1 -0.091501 0.287590 -0.000009
1 0.242708 -2.780223 0.000062

(5) charge and multiplicity: 1,3

8 8.815992 -0.710968 -0.059031
6 7.619010 -0.525607 -0.042253
7 6.683600 -1.471290 0.360652
7 7.002535 0.660263 -0.423511
7 5.338432 -1.310358 0.396248
7 5.671318 0.913488 -0.420860
6 4.911006 -0.106389 -0.003922
6 3.447973 0.120999 0.017705
6 2.574967 -0.892698 0.445005
6 2.911871 1.354114 -0.390626
6 1.204322 -0.678911 0.467468
6 1.542244 1.568540 -0.372006
6 0.663980 0.556573 0.063161
6 -0.778949 0.800627 0.093563
6 -1.396183 1.998921 0.290220
16 -1.883579 -0.556042 -0.159576
16 -3.125496 2.060601 0.288342
6 -3.364292 0.352796 0.027999
6 -4.626352 -0.233448 -0.038079
16 -4.858506 -1.950364 -0.290852
16 -6.111281 0.681634 0.122983
6 -6.601696 -1.892551 -0.245585
6 -7.173609 -0.690637 -0.056437
1 7.036122 -2.371464 0.659173
1 7.602199 1.413564 -0.734477
1 3.581712 2.133511 -0.733045
1 1.148345 2.514965 -0.728253
1 0.554117 -1.468229 0.833765
1 -0.875437 2.927366 0.489215
1 -7.135379 -2.826770 -0.372701
1 -8.239896 -0.505008 -0.007736
1 2.985116 -1.842126 0.766992

(6) charge and multiplicity: 1,3

8 6.704912 -3.080058 0.431445
6 5.915206 -2.170603 0.298828
7 4.539444 -2.300130 0.446957
7 6.263699 -0.864884 -0.021066
7 3.615067 -1.315909 0.309186
7 5.414652 0.180536 -0.175719
6 4.123658 -0.116523 0.001484
6 3.156277 0.998563 -0.159784
6 1.787471 0.773220 0.016739
6 3.600696 2.289774 -0.481805
6 0.866721 1.822016 -0.126775
6 2.688084 3.333565 -0.628254
6 1.325866 3.110608 -0.457738
6 -0.569937 1.587985 0.067457
6 -1.479230 2.473879 0.555777
16 -1.244104 0.019368 -0.382879

16 -3.136458 1.984505 0.686784
6 -2.889568 0.366743 0.084324
6 -3.921888 -0.564577 -0.027837
16 -3.669268 -2.188162 -0.630267
16 -5.576316 -0.207704 0.419391
6 -5.332195 -2.688222 -0.467690
6 -6.203564 -1.783281 0.012173
1 4.187730 -3.218271 0.683849
1 7.247404 -0.665570 -0.149015
1 4.661497 2.462936 -0.617961
1 3.042021 4.325360 -0.889277
1 0.620241 3.920593 -0.611136
1 -1.234177 3.468523 0.907227
1 -5.579903 -3.701186 -0.761562
1 -7.262594 -1.953298 0.165092
1 1.461186 -0.222902 0.295864

(7) charge and multiplicity: 1,3

8 -3.922772 -6.862410 -0.000000
6 -3.706380 -5.670482 -0.000000
7 -2.437525 -5.103367 -0.000000
7 -4.693286 -4.692621 -0.000000
7 -2.136379 -3.779426 -0.000000
7 -4.492555 -3.352533 -0.000000
6 -3.208468 -2.980282 -0.000000
6 -2.965640 -1.510190 -0.000000
7 -1.696332 -1.101906 -0.000000
6 -4.044443 -0.604796 -0.000000
6 -1.441535 0.214700 -0.000000
6 -3.771012 0.756639 -0.000000
6 -2.444338 1.189494 -0.000000
6 -0.000000 0.536591 0.000000
6 0.979203 -0.405888 0.000000
16 0.562709 2.202876 0.000000
16 2.624433 0.118133 0.000000
6 2.268018 1.826152 0.000000
6 3.257914 2.809040 0.000000
16 2.893330 4.520261 0.000000
16 4.967203 2.432973 0.000000
6 4.556126 5.046474 0.000000
6 5.503730 4.092290 0.000000
1 -1.651431 -5.739989 -0.000000
1 -5.656244 -5.003035 -0.000000
1 -5.059477 -0.980788 -0.000000
1 -4.581133 1.478298 -0.000000
1 -2.213904 2.250372 -0.000000
1 0.760661 -1.467688 0.000000
1 4.742037 6.113825 0.000000
1 6.572350 4.270911 0.000000

(8) charge and multiplicity: 1,3
O 8.242019 -1.019491 -0.273809
C 7.105709 -0.613288 -0.182238
N 6.760543 0.721335 0.008238
N 5.977583 -1.425827 -0.254741
N 5.507972 1.224179 0.115198
N 4.688466 -1.017999 -0.156573
C 4.542627 0.303043 0.024523
C 3.170756 0.779860 0.131081
N 2.122271 -0.089356 0.054439
C 0.932225 0.604498 0.158306
C 2.657748 2.069386 0.302948
C 1.263586 1.960827 0.316938
C -0.348319 -0.032504 0.128192
C -0.611858 -1.371033 0.265642
S -1.780577 0.977171 -0.121840
S -2.250576 -1.904801 0.213695
C -2.956733 -0.321454 0.014111
C -4.324278 -0.105909 -0.048849
S -5.019722 1.494247 -0.236953
S -5.506761 -1.400432 0.051309
C -6.682710 0.957679 -0.218126
C -6.904166 -0.360207 -0.086666
H 7.518047 1.389718 0.072780
H 6.130907 -2.416352 -0.392702
H 0.135903 -2.131422 0.453964
H -7.451173 1.715094 -0.314424
H -7.878960 -0.832079 -0.060858
H 3.251167 2.964174 0.410084
H 2.256152 -1.072185 -0.137318
H 0.558617 2.768298 0.458470

(9) charge and multiplicity: 1,3
8 -2.680587 -7.728457 0.000000
6 -2.576873 -6.522715 0.000000
7 -3.655426 -5.642802 0.000000
7 -1.364070 -5.840267 0.000000
7 -3.589619 -4.291214 0.000000
7 -1.192170 -4.495766 0.000000
6 -2.338688 -3.807016 0.000000
6 -2.248370 -2.353660 0.000000
8 -1.013857 -1.787144 0.000000
6 -1.193472 -0.430136 0.000000
6 -3.222220 -1.376480 0.000000
6 -2.544480 -0.138488 0.000000
6 -0.002328 0.361633 0.000000
6 1.272254 -0.136591 0.000000
16 -0.125645 2.121504 0.000000
16 2.584507 0.978195 0.000000
6 1.605412 2.422808 0.000000

6 2.142573 3.702646 0.000000
16 1.145917 5.145215 0.000000
16 3.868783 4.017020 0.000000
6 2.480534 6.271974 0.000000
6 3.721300 5.757235 0.000000
1 -4.583341 -6.047179 0.000000
1 -0.520855 -6.399651 0.000000
1 1.503684 -1.194678 0.000000
1 2.240563 7.328360 0.000000
1 4.638550 6.333709 0.000000
1 -4.286941 -1.550754 0.000000
1 -2.992827 0.845270 0.000000

(10) charge and multiplicity: 1,3
O 8.562985 -0.325939 -0.200198
C 7.368237 -0.144398 -0.131860
N 6.414770 -1.151662 -0.244224
N 6.773719 1.097650 0.069188
N 5.071602 -0.995063 -0.172393
N 5.446127 1.354100 0.151176
C 4.672822 0.268076 0.022379
C 3.231131 0.485964 0.101220
S 2.130606 -0.848554 -0.077917
C 2.566286 1.680933 0.303408
C 0.753696 0.218875 0.135868
C 1.166974 1.530999 0.322440
C -0.593343 -0.286764 0.109677
C -0.983745 -1.594145 0.211442
S -1.928205 0.861131 -0.089259
S -2.666693 -1.968437 0.162985
C -3.218018 -0.321000 0.010920
C -4.562662 0.025848 -0.040534
S -5.104201 1.686706 -0.182054
S -5.858464 -1.153751 0.029262
C -6.808790 1.308794 -0.174851
C -7.152348 0.013382 -0.078123
H 6.751221 -2.094691 -0.391063
H 7.390438 1.894765 0.162418
H 3.090353 2.618152 0.437135
H 0.483735 2.356357 0.491008
H -0.303009 -2.426017 0.347974
H -7.503264 2.136881 -0.249420
H -8.167008 -0.365977 -0.06291

BS-UB3LYP/6-31G(d,p) optimized geometries

(1) charge and multiplicity: 1,1
8 -6.378569 -0.909026 0.000448
6 -5.218341 -0.575492 -0.000309
7 -4.142440 -1.459689 0.000078

7 -4.786612 0.754695 -0.000028
7 -2.832182 -1.119052 0.000057
7 -3.507855 1.182177 -0.000069
6 -2.607747 0.196127 -0.000117
6 -1.195421 0.598156 -0.000124
6 -0.724127 1.866733 -0.000159
16 0.000770 -0.686895 -0.000088
16 0.995410 2.087947 -0.000178
6 1.382968 0.381702 -0.000021
6 2.696980 -0.089059 0.000049
16 3.093237 -1.792888 0.000160
16 4.084592 0.976235 0.000019
6 4.820883 -1.563808 0.000114
6 5.274574 -0.297064 0.000054
1 -4.352422 -2.450229 0.000402
1 -5.502069 1.472068 0.000237
1 -1.356591 2.746084 -0.000190
1 5.442421 -2.451308 0.000140
1 6.318074 -0.005476 0.000022

(2) charge and multiplicity: 1,1

8 -7.752896 -0.543058 0.000230
6 -6.546764 -0.447456 -0.000002
7 -5.674568 -1.534100 0.000141
7 -5.853321 0.758461 -0.000119
7 -4.325771 -1.478567 0.000140
7 -4.507324 0.916220 -0.000112
6 -3.821006 -0.240726 -0.000001
6 -2.362714 -0.175980 -0.000020
6 -1.657825 0.974587 -0.000025
6 -0.216288 1.078540 -0.000031
6 0.474876 2.255154 -0.000095
16 0.801200 -0.367854 0.000075
16 2.204332 2.211009 -0.000091
6 2.333355 0.471157 -0.000016
6 3.556930 -0.196459 -0.000012
16 3.681859 -1.942130 -0.000036
16 5.095482 0.639081 -0.000004
6 5.425161 -1.985862 -0.000009
6 6.071029 -0.806092 -0.000012
1 -6.087067 -2.458682 0.000345
1 -6.405835 1.606626 -0.000099
1 -1.881106 -1.150423 -0.000023
1 -2.195623 1.918694 -0.000031
1 0.005810 3.231903 -0.000155
1 5.900123 -2.959650 -0.000004
1 7.147264 -0.680977 -0.000010

(3) charge and multiplicity: 1,1

8 -4.261809 8.034476 0.000000

6 -3.632957 6.999553 0.000000
7 -2.242208 6.928335 0.000000
7 -4.203522 5.732557 0.000000
7 -1.496349 5.802668 0.000000
7 -3.544291 4.547308 0.000000
6 -2.202556 4.665648 0.000000
6 -1.403240 3.446973 0.000000
6 -1.910798 2.190277 0.000000
6 -1.076462 1.025334 0.000000
6 -1.555772 -0.248710 0.000000
6 -0.768337 -1.451754 0.000000
6 -1.287246 -2.719036 0.000000
16 1.001167 -1.391361 0.000000
16 -0.209577 -4.067436 0.000000
6 1.257657 -3.123569 0.000000
6 2.524422 -3.696251 0.000000
16 3.994100 -2.741689 0.000000
16 2.788053 -5.429712 0.000000
6 5.081376 -4.107541 0.000000
6 4.530939 -5.333519 0.000000
1 -1.734728 7.804206 0.000000
1 -5.214379 5.683960 0.000000
1 -0.329669 3.614340 0.000000
1 -2.989379 2.055423 0.000000
1 -2.348660 -2.936314 0.000000
1 6.144359 -3.898600 0.000000
1 5.080847 -6.266939 0.000000
1 0.000000 1.198978 0.000000
1 -2.631388 -0.408187 0.000000

(4) charge and multiplicity: 1,1

8 9.784711 3.609708 0.000000
6 8.610300 3.311444 0.000000
7 7.569223 4.236058 0.000000
7 8.129264 2.009236 0.000000
7 6.247583 3.957386 0.000000
7 6.827034 1.625583 0.000000
6 5.953310 2.651022 0.000000
6 4.529640 2.342308 0.000000
6 4.008292 1.089217 0.000000
6 2.599744 0.844516 0.000000
6 2.035309 -0.401730 0.000000
6 0.627786 -0.616648 0.000000
6 0.042121 -1.852020 0.000000
6 -1.363789 -2.122072 0.000000
6 -1.909305 -3.381827 0.000000
16 -2.559940 -0.814014 0.000000
16 -3.622914 -3.555407 0.000000
6 -3.980085 -1.846144 0.000000
6 -5.272726 -1.346339 0.000000

16 -5.622095 0.373716 0.000000
16 -6.697752 -2.372924 0.000000
6 -7.360249 0.191684 0.000000
6 -7.849487 -1.058807 0.000000
1 7.823881 5.215629 0.000000
1 8.814845 1.265093 0.000000
1 3.880630 3.213633 0.000000
1 4.683820 0.237545 0.000000
1 -1.321601 -4.291994 0.000000
1 -7.955575 1.096643 0.000000
1 -8.900828 -1.319874 0.000000
1 1.943051 1.714564 0.000000
1 2.683538 -1.276223 0.000000
1 -0.000000 0.274886 0.000000
1 0.676885 -2.734968 0.000000

(5) charge and multiplicity: 1,1
8 8.815467 -0.716546 -0.072159
6 7.619331 -0.526789 -0.052280
7 6.683365 -1.464687 0.370992
7 7.002292 0.653103 -0.447965
7 5.340640 -1.300429 0.411702
7 5.670815 0.908374 -0.442302
6 4.911464 -0.103767 -0.004938
6 3.446904 0.122987 0.021643
6 2.577018 -0.883965 0.468653
6 2.908875 1.348796 -0.403370
6 1.205845 -0.670168 0.494813
6 1.538619 1.563224 -0.381439
6 0.663781 0.558265 0.074043
6 -0.780432 0.803725 0.107563
6 -1.398123 2.000810 0.303152
16 -1.882300 -0.554579 -0.144597
16 -3.129594 2.061018 0.295340
6 -3.364023 0.352284 0.033867
6 -4.625419 -0.235651 -0.040396
16 -4.855449 -1.951855 -0.298696
16 -6.111156 0.678424 0.115587
6 -6.598616 -1.894575 -0.263875
6 -7.172008 -0.693209 -0.074464
1 7.036129 -2.360775 0.681786
1 7.600857 1.401122 -0.773508
1 3.576574 2.123147 -0.761181
1 1.142079 2.503896 -0.749866
1 0.557641 -1.453988 0.876176
1 -0.878600 2.929836 0.502496
1 -7.131392 -2.828503 -0.396875
1 -8.238640 -0.508163 -0.031313
1 2.988529 -1.828663 0.802602

(6) charge and multiplicity: 1,1
8 6.708555 -3.075789 0.422013
6 5.917428 -2.167832 0.293819
7 4.541909 -2.296539 0.448165
7 6.262994 -0.860124 -0.027094
7 3.618191 -1.313719 0.314756
7 5.414407 0.182567 -0.176038
6 4.123361 -0.112959 0.004994
6 3.156376 1.002013 -0.153664
6 1.787260 0.773617 0.017044
6 3.601615 2.294286 -0.468396
6 0.865504 1.822073 -0.123996
6 2.687856 3.337705 -0.612770
6 1.325603 3.112358 -0.447621
6 -0.571434 1.585887 0.065763
6 -1.480411 2.471108 0.554688
16 -1.245244 0.017367 -0.388989
16 -3.137836 1.982798 0.685947
6 -2.891982 0.364093 0.081451
6 -3.922849 -0.565915 -0.029472
16 -3.670238 -2.191054 -0.631412
16 -5.578609 -0.209209 0.418139
6 -5.333591 -2.691246 -0.466566
6 -6.204770 -1.786389 0.012875
1 4.190827 -3.214633 0.687608
1 7.246404 -0.660024 -0.159170
1 4.662417 2.469708 -0.601161
1 3.041390 4.331050 -0.868374
1 0.619867 3.922455 -0.599724
1 -1.234838 3.465119 0.907638
1 -5.581297 -3.704515 -0.759239
1 -7.263584 -1.956870 0.166538
1 1.460310 -0.223896 0.289969

(7) charge and multiplicity: 1,1
8 -3.899924 -6.878525 -0.000000
6 -3.686811 -5.686886 -0.000000
7 -2.419517 -5.113812 -0.000000
7 -4.676402 -4.709755 -0.000000
7 -2.123844 -3.791828 -0.000000
7 -4.479405 -3.372561 -0.000000
6 -3.197053 -2.993455 -0.000000
6 -2.959175 -1.523037 -0.000000
7 -1.690527 -1.112953 -0.000000
6 -4.041252 -0.622961 -0.000000
6 -1.438649 0.204706 0.000000
6 -3.771088 0.739882 0.000000
6 -2.446218 1.175852 0.000000
6 0.000000 0.534273 0.000000
6 0.984102 -0.402384 -0.000000

16 0.552800 2.205486 0.000000
16 2.627086 0.128624 0.000000
6 2.262723 1.837105 0.000000
6 3.246003 2.822801 0.000000
16 2.872346 4.533910 0.000000
16 4.959285 2.456334 0.000000
6 4.533382 5.068441 0.000000
6 5.485840 4.119726 0.000000
1 -1.630816 -5.747918 -0.000000
1 -5.638890 -5.023109 -0.000000
1 -5.055367 -1.001115 -0.000000
1 -4.582939 1.459610 0.000000
1 -2.218923 2.237350 0.000000
1 0.771976 -1.465381 -0.000000
1 4.713731 6.136706 0.000000
1 6.553395 4.304406 0.000000

(8) charge and multiplicity: 1,1
8 -7.285287 -2.405390 -0.213094
6 -6.351758 -1.638162 -0.142000
7 -5.017785 -2.015349 -0.254350
7 -6.476719 -0.266249 0.062242
7 -3.941607 -1.191711 -0.179864
7 -5.468621 0.631350 0.147906
6 -4.251007 0.096999 0.019888
6 -3.122111 1.017572 0.104375
7 -1.841759 0.559272 -0.006529
6 -3.076621 2.402485 0.280546
6 -0.958450 1.619082 0.075667
6 -1.729424 2.779154 0.261619
6 0.463659 1.475622 0.004939
6 1.359338 2.489925 -0.218816
16 1.202958 -0.114492 0.244610
16 3.042149 2.119328 -0.253005
6 2.863181 0.400405 -0.006387
6 3.934476 -0.478965 0.009978
16 3.739961 -2.205061 0.257773
16 5.598190 0.036073 -0.212825
6 5.441829 -2.584886 0.138105
6 6.287294 -1.563961 -0.075967
1 -4.827277 -2.997252 -0.405722
1 -7.414644 0.103227 0.155428
1 -3.937183 3.040068 0.411974
1 -1.339079 3.777094 0.400973
1 1.078539 3.518871 -0.404698
1 5.728632 -3.624059 0.244269
1 7.363096 -1.650838 -0.169212
1 -1.638930 -0.410356 -0.210629

(9) charge and multiplicity: 1,1

8 8.082211 -1.258836 -0.000001
6 6.967698 -0.786749 0.000022
7 5.796422 -1.535913 0.000323
7 6.696197 0.579458 -0.000317
7 4.527382 -1.055682 0.000369
7 5.472800 1.154500 -0.000534
6 4.458744 0.279228 -0.000129
6 3.131893 0.886666 -0.000063
8 2.053598 0.061749 -0.000129
6 2.727106 2.203572 0.000085
6 0.939025 0.856877 -0.000003
6 1.313703 2.185339 0.000103
6 -0.317754 0.170792 -0.000025
6 -0.474466 -1.188111 0.000076
16 -1.813338 1.102904 -0.000217
16 -2.077386 -1.824723 0.000090
6 -2.890614 -0.281010 -0.000071
6 -4.274756 -0.153615 -0.000045
16 -5.082876 1.401456 0.000141
16 -5.358753 -1.531609 -0.000048
6 -6.702443 0.749356 0.000194
6 -6.827694 -0.588545 0.000131
1 5.893697 -2.543009 0.000682
1 7.488625 1.209357 -0.000720
1 3.379921 3.062476 0.000162
1 0.655245 3.042830 0.000233
1 0.351549 -1.888449 0.000189
1 -7.523953 1.455574 0.000303
1 -7.766158 -1.129870 0.000183

(10) charge and multiplicity: 1,1
8 8.563842 -0.321909 -0.210575
6 7.368536 -0.144353 -0.140209
7 6.416038 -1.150267 -0.256741
7 6.772197 1.096970 0.068489
7 5.071411 -0.994722 -0.182461
7 5.446021 1.350786 0.153483
6 4.673069 0.266889 0.020065
6 3.229645 0.487574 0.103797
16 2.130012 -0.846887 -0.073556
6 2.566049 1.680843 0.308939
6 0.752949 0.219387 0.144774
6 1.165059 1.530012 0.331924
6 -0.594008 -0.291088 0.120864
6 -0.984413 -1.597729 0.221581
16 -1.927132 0.856893 -0.075407
16 -2.670545 -1.970850 0.168254
6 -3.216973 -0.321862 0.016110
6 -4.562188 0.028048 -0.042125
16 -5.102031 1.688182 -0.188674

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16 -5.857669 -1.150628 0.024225
6 -6.806185 1.311161 -0.189933
6 -7.150644 0.015665 -0.092441
1 6.752229 -2.092385 -0.409330
1 7.388461 1.894097 0.165530
1 3.089401 2.618588 0.441475
1 0.482456 2.355405 0.503168
1 -0.304883 -2.430402 0.358087
1 -7.500080 2.139286 -0.269677
1 -8.165519 -0.363319 -0.081591