An Electron Transfer Driven Magnetic Switch: Ferromagnetic Exchange and Spin Delocalization in Iron Verdazyl Complexes.

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Supporting Information

Figure S1: IR spectra for $[Fe(dipyvd)_2]^+PF_6^-$ (blue) and $[Fe(dipyvd)_2]^{2+}(PF_6^-)_2$ (red). Lower figure is an expansion of the fingerprint region

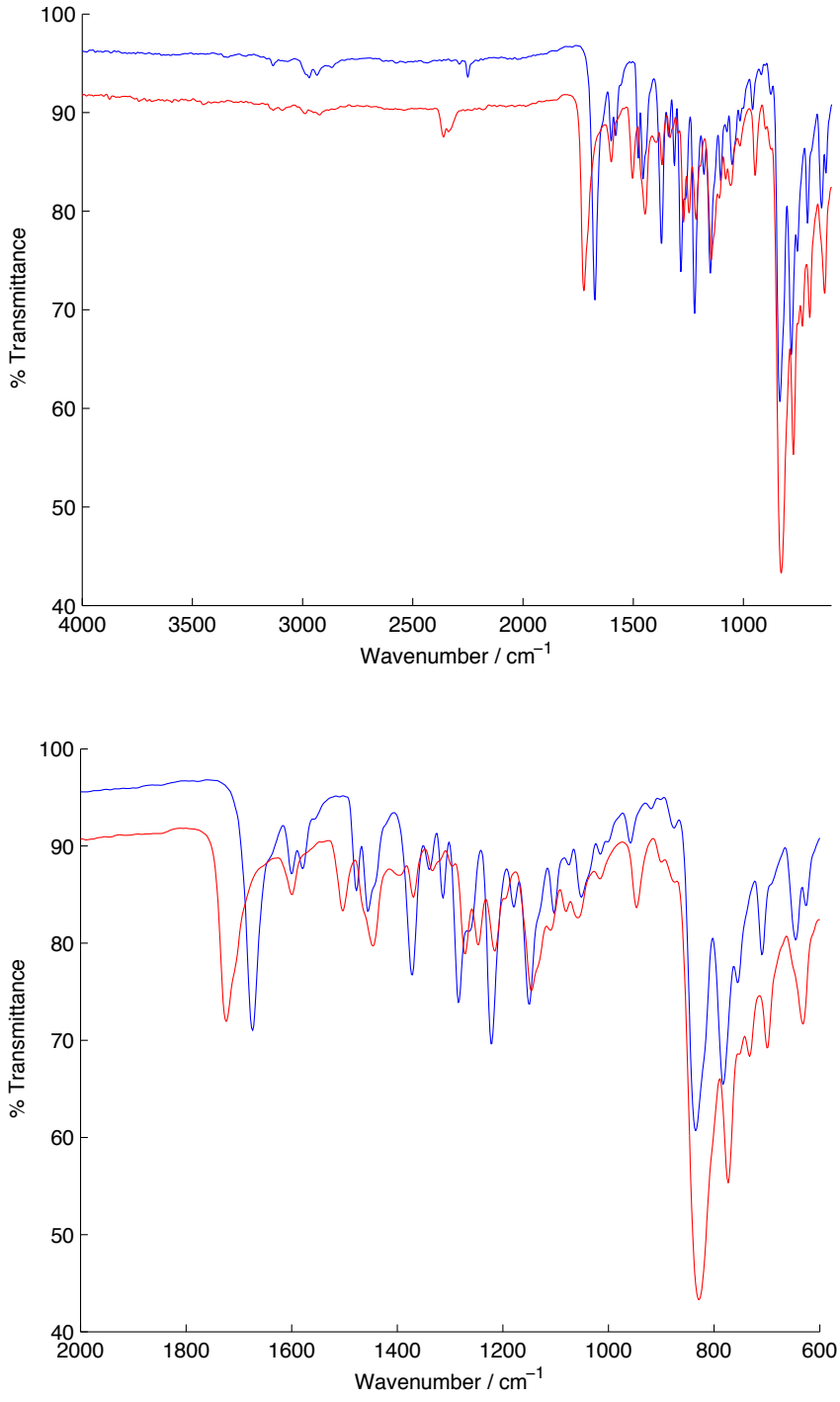


Figure S2: Spectroelectrochemical data for $[Fe(dipyvd)_2]^{n+}$ in acetonitrile. Spectra recorded at –1.0 V ($[Fe(dipyvd)_2]^0$, cyan), +0.16 V ($[Fe(dipyvd)_2]^{1+}$, blue), +0.56 V ($[Fe(dipyvd)_2]^{2+}$, green) and +1.26 V ($[Fe(dipyvd)_2]^{3+}$, red). Potentials reported vs. SCE.

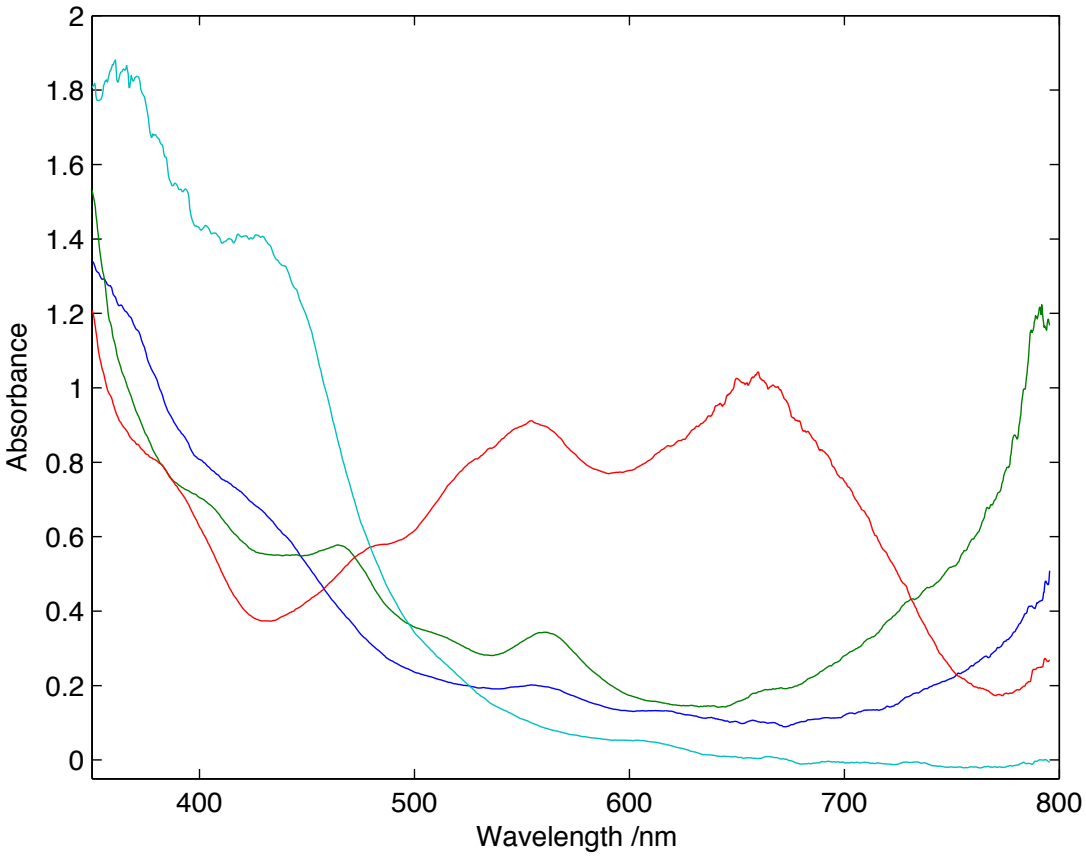


Figure S3. ^{1}H NMR and ^{13}C NMR spectra of **2**

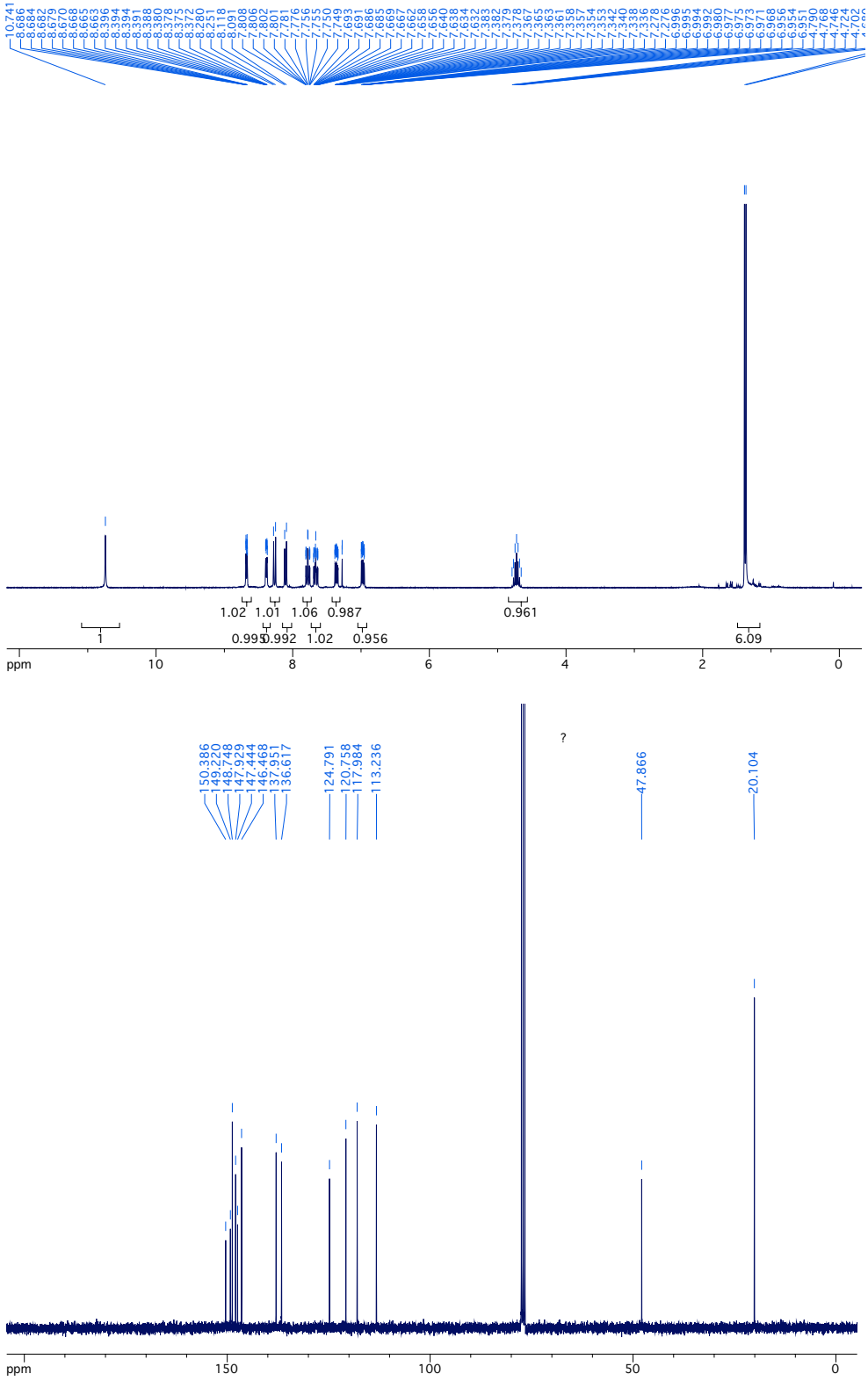
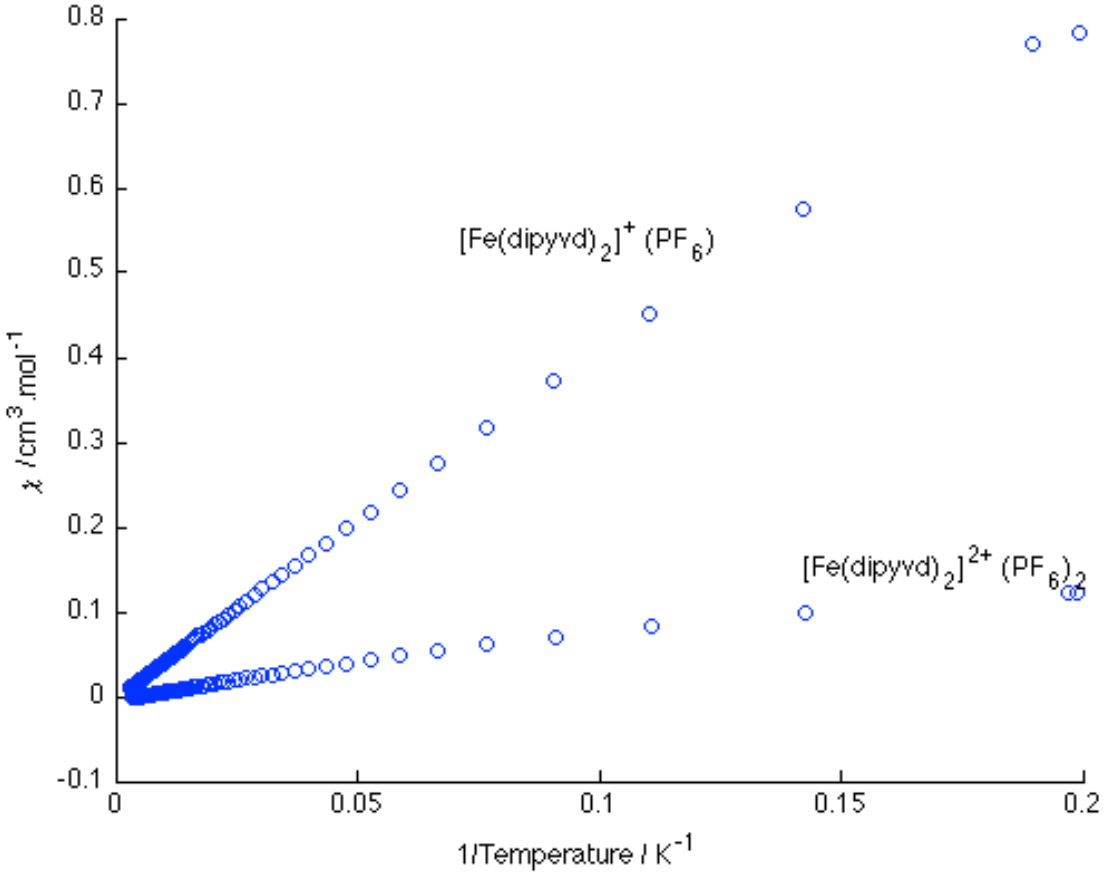


Figure S4. Plot of χ vs $1/T$. for $[Fe(dipyvd)_2]^+ PF_6^-$ and $[Fe(dipyvd)_2]^{2+} (PF_6^-)_2$



S5. Results from DFT calculations

A. $[Fe(dipyvd)_2]^+$, S=5/2

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--------------------------------
CARTESIAN COORDINATES (ANGSTROEM)
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  Fe     8.186200    8.186199    3.484777
  O     11.639875    4.456534    1.924083
  N      9.941629    7.199865    3.490231
  N     10.174940    6.103943    2.647277
  N     12.352944    5.917403    3.544526
  N     12.151242    6.989608    4.377898
  N      9.427529    9.230982    5.005418
  N      8.007203    6.598185    2.011963
  C     11.421023    5.413321    2.651208
  C     10.972979    7.553645    4.296825
  C     10.671015    8.713221    5.158660
  C     11.589971    9.247094    6.068500
  H     12.576660    8.794337    6.151762
  C     11.210136   10.342937    6.838200
  H     11.906934   10.779292    7.554584
  C      9.926343   10.876789    6.680846
  H      9.592864   11.734073    7.264636
  C      9.069632   10.290661    5.754006
  H      8.059669   10.671422    5.593444
  C      6.893536    6.381538    1.277136
  H      6.068219    7.069604    1.466127
  C      6.788268    5.364570    0.345230
  H      5.869246    5.231032   -0.223232
  C      7.898498    4.526111    0.163844
  H      7.863422    3.711248   -0.560051
  C      9.054464    4.724019    0.902750
  H      9.926188    4.090985    0.781460
  C      9.081530    5.784263    1.834262
  C     13.697271    5.284224    3.639771
  H     13.658260    4.464094    2.913083
  C     14.780323    6.282953    3.226817
  H     14.616096    6.648329    2.203714
  H     15.762190    5.791864    3.257885
  H     14.804217    7.143110    3.909592
  C     13.913600    4.715143    5.043314
  H     13.905241    5.513162    5.798052
  H     14.888232    4.210820    5.087084
  H     13.139002    3.978858    5.298558
  O      4.732527   11.915865    1.924083
  N      6.430770    9.172534    3.490230
  N      6.197460   10.268456    2.647277
  N      4.019458   10.454998    3.544526
  N      4.221159    9.382792    4.377898
  N      6.944870    7.141416    5.005417
  N      8.365198    9.774214    2.011963
  C      4.951378   10.959077    2.651208
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```
  C      5.399421    8.818755    4.296823
  C      5.701384    7.659179    5.158659
  C      4.782427    7.125308    6.068497
  H      3.795739    7.578066    6.151757
  C      5.162258    6.029464    6.838198
  H      4.465458    5.593110    7.554582
  C      6.446050    5.495609    6.680846
  H      6.779528    4.638325    7.264636
  C      7.302764    6.081736    5.754006
  H      8.312726    5.700974    5.593446
  C      9.478864    9.990861    1.277135
  H     10.304182    9.302796    1.466125
  C      9.584133   11.007830    0.345229
  H     10.503154   11.141368   -0.223233
  C      8.473901   11.846288    0.163844
  H      8.508976   12.661151   -0.560052
  C      7.317936   11.648379    0.902750
  H      6.446211   12.281412    0.781460
  C      7.290870   10.588136    1.834262
  C      2.675133   11.088177    3.639772
  H      2.714143   11.908307    2.913083
  C      1.592078   10.089450    3.226820
  H      1.756304    9.724073    2.203717
  H      0.610212   10.580539    3.257890
  H      1.568187    9.229293    3.909596
  C      2.458806   11.657259    5.043315
  H      2.467166   10.859241    5.798053
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  H      3.233404   12.393544    5.298557


-------------------------------------------
MULLIKEN ATOMIC CHARGES AND SPIN POPULATIONS
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   0 Fe:    0.451060    3.961987
   1 O :   -0.381803    0.003195
   2 N :   -0.201281    0.185412
   3 N :    0.011490    0.053906
   4 N :    0.017189    0.057301
   5 N :   -0.235834    0.168939
   6 N :   -0.167288    0.029367
   7 N :   -0.198935    0.072573
   8 C :    0.342609   -0.002684
   9 C :    0.112738   -0.067541
  10 C :    0.182145    0.009967
  11 C :   -0.182540   -0.007393
  12 H :    0.163439    0.000615
  13 C :   -0.062829    0.002181
  14 H :    0.152458   -0.000079
  15 C :   -0.104266   -0.008253
  16 H :    0.147746    0.001586
  17 C :   -0.072588    0.001782
  18 H :    0.146887    0.002643
```

19	C	:	-0.073106	-0.014927
20	H	:	0.144018	0.003729
21	C	:	-0.120137	0.029594
22	H	:	0.142003	-0.000182
23	C	:	-0.077797	-0.013357
24	H	:	0.150400	0.000423
25	C	:	-0.189043	0.025862
26	H	:	0.195602	0.000347
27	C	:	0.230689	-0.017514
28	C	:	0.049345	-0.003856
29	H	:	0.132284	0.000112
30	C	:	-0.350067	0.003096
31	H	:	0.115905	0.000043
32	H	:	0.126073	-0.000268
33	H	:	0.119175	-0.000211
34	C	:	-0.349457	0.003029
35	H	:	0.119100	-0.000208
36	H	:	0.125794	-0.000269
37	H	:	0.114285	0.000049
38	O	:	-0.381823	0.003195
39	N	:	-0.201314	0.185413
40	N	:	0.011211	0.053905
41	N	:	0.017428	0.057299
42	N	:	-0.235574	0.168933
43	N	:	-0.167162	0.029361
44	N	:	-0.198861	0.072573
45	C	:	0.342227	-0.002685
46	C	:	0.112785	-0.067553
47	C	:	0.182020	0.009985
48	C	:	-0.182944	-0.007394
49	H	:	0.163440	0.000615
50	C	:	-0.062552	0.002179
51	H	:	0.152463	-0.000078
52	C	:	-0.104372	-0.008250
53	H	:	0.147714	0.001587
54	C	:	-0.072517	0.001784
55	H	:	0.146946	0.002642
56	C	:	-0.072966	-0.014923
57	H	:	0.144009	0.003728
58	C	:	-0.120255	0.029589
59	H	:	0.142012	-0.000182
60	C	:	-0.077732	-0.013353
61	H	:	0.150399	0.000424
62	C	:	-0.189306	0.025856
63	H	:	0.195590	0.000347
64	C	:	0.231123	-0.017513
65	C	:	0.049475	-0.003857
66	H	:	0.132277	0.000112
67	C	:	-0.350081	0.003096
68	H	:	0.115907	0.000043
69	H	:	0.126074	-0.000268
70	H	:	0.119178	-0.000211
71	C	:	-0.349456	0.003030
72	H	:	0.119099	-0.000208

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  73 H :    0.125795   -0.000269
  74 H :    0.114282    0.000049
Sum of atomic charges         :    1.0000000
Sum of atomic spin populations:    5.0000000
```

ABSORPTION SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS

State	Energy (cm-1)	Wavelength (nm)	fosc	T2 (au**2)	TX (au)	TY (au)	TZ (au)
1	7009.0	1426.7	0.002708706	0.12723	-0.00150	0.35669	0.00014
2	7109.3	1406.6	0.001755911	0.08131	0.00001	0.00017	-0.28515
3	8458.9	1182.2	0.000137937	0.00537	0.00000	0.00000	-0.07327
4	8829.5	1132.6	0.000236870	0.00883	-0.05665	0.07499	-0.00000
5	10229.2	977.6	0.168427655	5.42058	1.88948	-1.36031	-0.00000
6	15968.5	626.2	0.001049963	0.02165	0.00002	-0.00002	0.14713
7	16917.2	591.1	0.008715588	0.16961	-0.35592	0.20720	0.00000
8	16997.0	588.3	0.000022120	0.00043	0.00021	-0.00012	-0.02070
9	17317.7	577.4	0.014941359	0.28404	-0.44124	0.29891	0.00001
10	20771.1	481.4	0.018930737	0.30004	0.00000	-0.00003	-0.54776
11	21106.5	473.8	0.014273351	0.22263	0.05235	-0.46892	-0.00013
12	21332.0	468.8	0.003910617	0.06035	0.00007	-0.00026	0.24567
13	21495.2	465.2	0.051917639	0.79515	0.35790	-0.81673	-0.00004
14	21772.5	459.3	0.007916224	0.11970	0.00004	-0.00010	0.34597
15	21932.5	455.9	0.000529487	0.00795	0.00368	0.08907	0.00018
16	22001.6	454.5	0.000954117	0.01428	0.00000	0.00006	-0.11948
17	23444.2	426.5	0.000380875	0.00535	-0.00668	0.07283	-0.00002
18	23635.2	423.1	0.000222700	0.00310	0.00003	-0.00004	-0.05570
19	23832.8	419.6	0.002680169	0.03702	-0.18744	0.04344	-0.00001
20	23945.9	417.6	0.000161438	0.00222	0.00004	-0.00002	-0.04711
21	24831.3	402.7	0.000426070	0.00565	0.00013	0.00010	-0.07516
22	24836.0	402.6	0.000948650	0.01257	-0.10660	-0.03481	-0.00015
23	24976.9	400.4	0.028461579	0.37514	-0.51674	0.32882	0.00004
24	25018.3	399.7	0.000093741	0.00123	-0.00063	0.00040	-0.03511
25	25796.9	387.6	0.007923548	0.10112	-0.30523	-0.08916	0.00007
26	25860.3	386.7	0.011368108	0.14472	0.00013	0.00003	0.38042
27	25951.2	385.3	0.013505110	0.17132	-0.06805	-0.40828	0.00008
28	26098.7	383.2	0.004517206	0.05698	-0.00002	0.00011	0.23871
29	26522.2	377.0	0.004418887	0.05485	-0.17131	0.15970	-0.00078
30	26523.7	377.0	0.000067842	0.00084	0.00463	-0.00434	-0.02832
31	26658.4	375.1	0.004489117	0.05544	-0.22197	-0.07853	0.00012
32	26709.2	374.4	0.001412797	0.01741	0.00006	-0.00004	0.13196
33	26735.5	374.0	0.000616971	0.00760	0.01466	0.08592	0.00012
34	26765.7	373.6	0.002634427	0.03240	-0.00005	0.00001	-0.18001
35	27389.4	365.1	0.011376255	0.13674	-0.36786	-0.03766	0.00015
36	27419.0	364.7	0.002096427	0.02517	0.00044	0.00004	0.15865
37	27472.9	364.0	0.003462634	0.04149	0.19158	-0.06839	-0.01057
38	27473.2	364.0	0.000449612	0.00539	0.03086	-0.01101	0.06568
39	27696.9	361.1	0.009291712	0.11044	-0.31610	0.10259	0.00001
40	27816.2	359.5	0.004392390	0.05199	-0.00002	0.00002	0.22800
41	27833.6	359.3	0.000410349	0.00485	0.00006	-0.00000	-0.06967
42	27962.5	357.6	0.035512444	0.41810	0.00074	0.00007	0.64661
43	27978.6	357.4	0.106712786	1.25564	1.11430	0.11819	-0.00045

```
  44   28136.7    355.4   0.000306791   0.00359  -0.05657  -0.01975  -0.00010
  45   28737.4    348.0   0.000066607   0.00076  -0.00007  -0.00001   0.02762
  46   28859.6    346.5   0.000161924   0.00185  -0.04297  -0.00070  -0.00003
  47   29485.2    339.2   0.004263291   0.04760   0.00119  -0.00169  -0.21817
  48   29494.3    339.0   0.020165028   0.22508   0.27339  -0.38773   0.00094
  49   30888.0    323.7   0.000019577   0.00021   0.00901  -0.01129   0.00000
  50   31479.1    317.7   0.084716041   0.88597  -0.93616  -0.09789   0.00026

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BROKEN SYMMETRY MAGNETIC COUPLING ANALYSIS
----------------------------------------

S(High-Spin)      =   2.5
<S**2>(High-Spin) =   8.8028
<S**2>(BrokenSym) =   4.1321
E(High-Spin)      = -3231.840103 Eh
E(BrokenSym)      = -3231.808769 Eh
E(High-Spin)-E(BrokenSym)= -0.8526 eV  -6876.424 cm**-1 (FERROMAGNETIC coupling)

          ---------------------------------------------------------
          | Spin-Hamiltonian Analysis based on H(HDvV)= -2J*SA*SB |
    -------                                                         -----------
    | J(1) =    1100.23 cm**-1    (from -(E[HS]-E[BS])/Smax**2)             |
    | J(2) =     785.88 cm**-1    (from -(E[HS]-E[BS])/(Smax*(Smax+1))      |
    | J(3) =    1472.24 cm**-1    (from -(E[HS]-E[BS])/(<S**2>HS-<S**2>BS)) |
    ---------------------------------------------------------------------------

  J(1): (a) A.P. Ginsberg J. Am. Chem. Soc. 102 (1980), 111
        (b) L. Noodleman J. Chem. Phys. 74 (1981), 5737
        (c) L. Noodleman E.R. Davidson Chem. Phys. 109 (1985), 131
  J(2)  (d) A. Bencini D. Gatteschi J. Am. Chem. Soc. 108 (1980), 5763
  J(3)  (e) K. Yamaguchi Y. Takahara T. Fueno in: V.H. Smith (Ed.)
            Applied Quantum Chemistry. Reidel, Dordrecht (1986), pp 155
        (f) T.Soda et al. Chem. Phys. Lett., 319, (2000), 223
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B. $[Fe(dipyvd)_2]^+$, S=3/2.

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CARTESIAN COORDINATES (ANGSTROEM)
--------------------------------
  Fe     8.186195    8.186202    3.494445
  O     11.489681    4.534658    1.880923
  N      9.830576    7.284226    3.477964
  N     10.041541    6.170672    2.641703
  N     12.243938    6.001628    3.480504
  N     12.044771    7.052479    4.339425
  N      9.293543    9.229166    5.024954
  N      7.861562    6.659509    2.112735
  C     11.293109    5.490727    2.614496
  C     10.873689    7.627549    4.291599
  C     10.560460    8.764148    5.168049
```

C	11.468784	9.325037	6.070109
H	12.472613	8.908421	6.139992
C	11.055499	10.401694	6.850270
H	11.740533	10.861332	7.562889
C	9.750357	10.884142	6.704526
H	9.388066	11.724353	7.296066
C	8.905099	10.270978	5.783462
H	7.879917	10.615188	5.639678
C	6.715328	6.448133	1.426377
H	5.895811	7.126979	1.662193
C	6.574270	5.442556	0.486270
H	5.629088	5.314799	-0.039062
C	7.674026	4.607501	0.239290
H	7.605850	3.803318	-0.493560
C	8.862132	4.799412	0.928087
H	9.731783	4.173062	0.762408
C	8.925149	5.845572	1.869844
C	13.593301	5.372917	3.547728
H	13.552634	4.575743	2.795877
C	14.666949	6.390798	3.159565
H	14.492922	6.789869	2.150847
H	15.651224	5.903730	3.165617
H	14.693731	7.227233	3.870899
C	13.821801	4.761188	4.931052
H	13.812542	5.534727	5.710820
H	14.800353	4.263155	4.953689
H	13.054892	4.010801	5.167360
O	4.882717	11.837745	1.880923
N	6.541817	9.088177	3.477964
N	6.330855	10.201731	2.641704
N	4.128459	10.370775	3.480505
N	4.327625	9.319925	4.339427
N	7.078858	7.143240	5.024946
N	8.510833	9.712886	2.112741
C	5.079288	10.881678	2.614499
C	5.498706	8.744854	4.291601
C	5.811940	7.608256	5.168048
C	4.903622	7.047363	6.070111
H	3.899792	7.463977	6.139999
C	5.316912	5.970705	6.850267
H	4.631882	5.511064	7.562888
C	6.622055	5.488260	6.704516
H	6.984350	4.648048	7.296052
C	7.467308	6.101427	5.783449
H	8.492489	5.757220	5.639660
C	9.657068	9.924258	1.426383
H	10.476583	9.245410	1.662200
C	9.798129	10.929834	0.486275
H	10.743313	11.057588	-0.039057
C	8.698376	11.764892	0.239293
H	8.766555	12.569074	-0.493558
C	7.510268	11.572985	0.928088
H	6.640620	12.199338	0.762409
C	7.447247	10.526827	1.869846

C	2.779096	10.999485	3.547727
H	2.819764	11.796659	2.795875
C	1.705450	9.981604	3.159563
H	1.879478	9.582531	2.150845
H	0.721174	10.468671	3.165613
H	1.678667	9.145169	3.870898
C	2.550593	11.611215	4.931050
H	2.559851	10.837677	5.710818
H	1.572041	12.109247	4.953685
H	3.317501	12.361602	5.167359

C. [Fe(dipyvd)2]+, S=1/2.

CARTESIAN COORDINATES (ANGSTROEM)

Fe	8.186199	8.186199	3.455022
O	11.387762	4.404145	2.117338
N	9.825342	7.309777	3.471621
N	9.972983	6.121690	2.748522
N	12.171686	5.986208	3.601432
N	12.005024	7.109403	4.397918
N	9.160706	9.284042	4.819622
N	7.860904	6.781331	2.090136
C	11.216528	5.419778	2.774056
C	10.841119	7.699187	4.266004
C	10.452636	8.884175	5.041486
C	11.290831	9.547584	5.937165
H	12.307693	9.179619	6.069479
C	10.801301	10.650777	6.632393
H	11.436714	11.185834	7.338257
C	9.482643	11.057434	6.410130
H	9.057165	11.913398	6.932821
C	8.699042	10.352734	5.500771
H	7.666504	10.638414	5.303603
C	6.755947	6.653858	1.320676
H	5.985882	7.407132	1.482463
C	6.591352	5.632888	0.399763
H	5.674252	5.571260	-0.183646
C	7.622521	4.692871	0.256722
H	7.529842	3.873211	-0.456178
C	8.772886	4.801213	1.022737
H	9.596626	4.099105	0.937804
C	8.875085	5.867151	1.936439
C	13.501149	5.327533	3.729808
H	13.444650	4.474043	3.043528
C	14.605714	6.281293	3.270986
H	14.450231	6.599977	2.231010
H	15.576523	5.770858	3.327613
H	14.647751	7.172783	3.911227
C	13.705608	4.821668	5.159414

H	13.712747	5.655029	5.874731
H	14.669730	4.300151	5.228303
H	12.916489	4.113596	5.448192
O	4.984636	11.968256	2.117335
N	6.547055	9.062622	3.471618
N	6.399414	10.250707	2.748515
N	4.200711	10.386190	3.601427
N	4.367372	9.262998	4.397916
N	7.211690	7.088358	4.819620
N	8.511497	9.591068	2.090136
C	5.155866	10.952617	2.774046
C	5.531276	8.673212	4.266003
C	5.919759	7.488224	5.041484
C	5.081564	6.824814	5.937162
H	4.064703	7.192779	6.069476
C	5.571095	5.721621	6.632389
H	4.935683	5.186563	7.338253
C	6.889753	5.314964	6.410126
H	7.315231	4.459000	6.932817
C	7.673355	6.019665	5.500768
H	8.705893	5.733986	5.303599
C	9.616456	9.718540	1.320680
H	10.386519	8.965265	1.482470
C	9.781053	10.739509	0.399767
H	10.698155	10.801136	-0.183640
C	8.749886	11.679527	0.256722
H	8.842567	12.499186	-0.456179
C	7.599518	11.571186	1.022733
H	6.775778	12.273295	0.937797
C	7.497316	10.505248	1.936435
C	2.871252	11.044870	3.729808
H	2.927749	11.898357	3.043526
C	1.766682	10.091110	3.270996
H	1.922158	9.772423	2.231020
H	0.795874	10.601548	3.327627
H	1.724647	9.199623	3.911240
C	2.666802	11.550738	5.159414
H	2.659665	10.717379	5.874733
H	1.702682	12.072257	5.228308
H	3.455924	12.258809	5.448186

D. $[Fe(dipyvd)_2]^{2+}$, S=0

CARTESIAN COORDINATES (ANGSTROEM)

Fe	2.311117	14.191637	11.418600
O	3.652847	18.437548	13.940395
N	2.056141	15.929837	11.990905
N	2.575148	12.448924	10.865366

N	1.744368	13.204546	13.045260
N	3.060978	9.923142	10.030485
N	2.931328	14.516507	9.532037
N	0.430723	14.498442	10.770331
N	1.595060	18.439478	12.886351
O	2.578569	9.133938	12.149420
N	3.007459	16.537343	12.782792
N	2.466150	11.417174	11.773472
N	0.631801	17.818020	12.160861
N	4.085010	14.572737	12.224214
N	3.227560	10.944072	9.152838
C	4.177955	15.773638	12.878793
C	5.349676	16.180134	13.534775
H	5.371495	17.136179	14.049026
C	2.964402	12.149303	9.604495
C	-0.037303	15.764366	11.000797
C	3.742605	14.626445	6.854441
H	4.057821	14.673977	5.812045
C	2.817790	17.875957	13.263990
C	1.954521	11.850511	13.003546
C	3.520467	15.795852	7.585738
H	3.657395	16.779118	7.136937
C	6.379076	14.126015	12.796634
H	7.226162	13.443603	12.745850
C	-1.305769	16.175159	10.593324
H	-1.624609	17.195126	10.805959
C	0.912065	16.606492	11.737269
C	-1.656407	13.970142	9.704089
H	-2.268479	13.225225	9.196695
C	-0.376579	13.626563	10.133810
H	0.021994	12.626290	9.969414
C	3.156882	13.371545	8.815825
C	3.115845	15.700907	8.915381
H	2.932458	16.593193	9.512583
C	3.558757	13.395049	7.481064
H	3.724613	12.451333	6.962329
C	6.455018	15.339606	13.489794
H	7.375450	15.635428	13.993264
C	1.260857	19.828360	13.351638
H	2.152181	20.140472	13.908467
C	2.693579	10.058090	11.372903
C	-2.129064	15.264654	9.933127
H	-3.126064	15.558754	9.604940
C	5.184895	13.786813	12.178508
H	5.077420	12.850584	11.633448
C	3.355441	8.551716	9.492268
H	3.168851	7.888991	10.345443
C	1.173987	13.725293	14.155633
H	1.005652	14.800821	14.143944
C	1.644440	11.010927	14.084025
H	1.838851	9.945420	14.007384
C	1.081364	11.579753	15.219658
H	0.833282	10.946002	16.071128
C	4.824909	8.462185	9.078073

H	5.047395	9.147569	8.249525
H	5.495889	8.683160	9.919344
H	5.036667	7.439125	8.741103
C	0.053453	19.784167	14.289302
H	-0.845457	19.434165	13.764634
H	0.239452	19.137111	15.157386
H	-0.142404	20.797486	14.663249
C	2.382972	8.223540	8.358934
H	1.338471	8.276506	8.694952
H	2.522197	8.901347	7.506139
H	2.572306	7.198730	8.014110
C	1.058116	20.741854	12.142489
H	1.949126	20.766182	11.500433
H	0.192128	20.425265	11.545995
H	0.872555	21.764016	12.497056
C	0.834035	12.956806	15.258850
H	0.397468	13.433715	16.135089

ABSORPTION SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS

State	Energy (cm-1)	Wavelength (nm)	fosc	T2 (au**2)	TX (au)	TY (au)	TZ (au)
1	9497.5	1052.9	0.013597378	0.47133	-0.02735	0.66238	0.17841
2	10504.9	951.9	0.000059378	0.00186	-0.01698	-0.00241	-0.03958
3	12283.9	814.1	0.000010673	0.00029	-0.00494	0.01474	-0.00667
4	12388.1	807.2	0.020481243	0.54428	0.03315	-0.71179	-0.19114
5	13084.8	764.2	0.000189491	0.00477	-0.00662	-0.05266	-0.04417
6	13722.6	728.7	0.099507255	2.38722	0.08531	-1.48516	-0.41744
7	15715.5	636.3	0.001014406	0.02125	0.08415	-0.08034	-0.08783
8	15988.5	625.4	0.000557360	0.01148	0.06564	-0.03984	0.07471
9	17245.8	579.8	0.000024801	0.00047	0.01026	0.00172	0.01911
10	17942.9	557.3	0.000053508	0.00098	-0.02013	0.01963	0.01382
11	18429.7	542.6	0.000660592	0.01180	-0.00843	-0.10570	-0.02358
12	18747.8	533.4	0.000087352	0.00153	-0.01657	0.02035	-0.02907
13	18992.7	526.5	0.005729092	0.09931	-0.13975	-0.28210	-0.01392
14	19303.8	518.0	0.017501589	0.29848	-0.29740	-0.45806	0.01461
15	19956.7	501.1	0.001183591	0.01952	-0.05595	0.05541	-0.11543
16	20012.4	499.7	0.012323694	0.20273	-0.20267	0.12044	-0.38360
17	21266.1	470.2	0.010800301	0.16720	0.19575	-0.12440	0.33675
18	21725.9	460.3	0.075958177	1.15099	0.67517	-0.79264	-0.25857
19	21831.1	458.1	0.035383756	0.53358	-0.12885	0.32390	0.64193
20	22357.0	447.3	0.001063128	0.01565	-0.10355	-0.03405	0.06143
21	22555.9	443.3	0.000327082	0.00477	-0.05774	0.00779	-0.03714
22	23490.4	425.7	0.002786715	0.03906	-0.17213	0.03336	0.09117
23	23622.2	423.3	0.001143276	0.01593	0.04914	-0.03202	0.11177
24	22263.3	449.2	0.000545328	0.00806	0.01501	-0.06587	0.05916
25	22427.6	445.9	0.000526828	0.00773	0.05026	0.02210	0.06870
26	25482.2	392.4	0.002208289	0.02853	0.12738	-0.05848	-0.09425
27	25549.8	391.4	0.002314819	0.02983	-0.13787	0.06023	0.08481
28	25898.6	386.1	0.001083127	0.01377	0.10885	0.03380	-0.02786
29	25771.4	388.0	0.005905738	0.07544	-0.03371	-0.06158	-0.26554
30	26087.5	383.3	0.023589083	0.29768	-0.22612	0.46096	0.18459
31	26353.2	379.5	0.000931385	0.01164	-0.03459	0.00916	-0.10176

32	26793.5	373.2	0.003547022	0.04358	-0.07785	0.03176	-0.19108
33	27268.7	366.7	0.003149422	0.03802	-0.00479	0.18256	0.06834
34	27395.4	365.0	0.005169469	0.06212	-0.13869	0.09233	-0.18537
35	27374.5	365.3	0.005665271	0.06813	0.23620	0.02408	-0.10845
36	27585.7	362.5	0.015506330	0.18505	-0.02752	-0.42083	-0.08486
37	28228.2	354.3	0.047319015	0.55186	-0.47127	0.44885	0.35818
38	28438.8	351.6	0.008007587	0.09270	-0.17869	0.11555	-0.21775
39	28609.4	349.5	0.003242117	0.03731	0.06528	-0.01744	0.18095
40	27770.5	360.1	0.002771899	0.03286	0.03927	-0.10322	-0.14375
41	27697.0	361.1	0.004158492	0.04943	-0.13982	0.10483	-0.13744
42	29484.4	339.2	0.007785626	0.08693	0.23900	0.13604	-0.10632
43	29855.7	334.9	0.001829447	0.02017	-0.06688	0.05676	-0.11171
44	29469.1	339.3	0.005961600	0.06660	-0.10233	0.05427	-0.23062
45	29533.8	338.6	0.023932678	0.26678	0.27459	-0.36289	-0.24430
46	30245.8	330.6	0.014551408	0.15839	0.20618	0.34023	0.01070
47	30416.9	328.8	0.002370702	0.02566	0.05010	0.02878	0.14940
48	30457.6	328.3	0.006010681	0.06497	0.04359	-0.25111	-0.00338
49	30403.3	328.9	0.002247482	0.02434	-0.02907	0.03178	0.14994
50	29949.0	333.9	0.012983334	0.14272	-0.28959	0.15569	0.18606

D. $[Fe(dipyvd)_2]^{2+}$, S=1

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CARTESIAN COORDINATES (ANGSTROEM)
--------------------------------
  Fe     2.320811   14.189460   11.430050
  O      3.740585   18.583700   13.661887
  N      2.050683   15.933967   11.997268
  N      2.589115   12.444757   10.864027
  N      1.738256   13.181808   13.042442
  N      3.014952    9.919710    9.985868
  N      3.002402   14.527525    9.569375
  N      0.419687   14.460140   10.833071
  N      1.585440   18.466187   12.833276
  O      2.282069    9.094700   12.017432
  N      3.060894   16.621991   12.638272
  N      2.312201   11.388346   11.708000
  N      0.589175   17.789896   12.205826
  N      4.095976   14.600755   12.225769
  N      3.290923   10.957610    9.155088
  C      4.225334   15.853822   12.763552
  C      5.413713   16.289877   13.367259
  H      5.467247   17.292919   13.779710
  C      3.067158   12.161880    9.629611
  C     -0.091245   15.694826   11.131435
  C      3.986149   14.668081    6.951691
  H      4.369598   14.727614    5.933117
  C      2.863137   17.964705   13.098128
  C      1.828474   11.818187   12.950121
  C      3.671896   15.828248    7.663807
  H      3.800890   16.816038    7.222844
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  C      6.367167   14.130438   12.866030
  H      7.191491   13.419250   12.886042
  C     -1.395392   16.060844   10.801206
  H     -1.746490   17.058049   11.064637
  C      0.866485   16.565212   11.820051
  C     -1.688329   13.878741    9.838083
  H     -2.288266   13.127687    9.325440
  C     -0.376227   13.577930   10.196040
  H      0.059033   12.605841    9.969008
  C      3.309546   13.391647    8.869406
  C      3.184233   15.718327    8.963897
  H      2.927411   16.603185    9.544433
  C      3.800841   13.430522    7.565237
  H      4.027470   12.493062    7.058416
  C      6.489716   15.411765   13.414840
  H      7.422536   15.730341   13.880100
  C      1.245186   19.863337   13.270580
  H      2.169149   20.224278   13.737548
  C      2.520912   10.034153   11.288552
  C     -2.208304   15.138652   10.144679
  H     -3.232151   15.398173    9.875507
  C      5.161263   13.768694   12.284922
  H      5.020474   12.783989   11.842989
  C      3.280818    8.551069    9.424244
  H      2.992282    7.873743   10.236633
  C      1.277653   13.713182   14.198290
  H      1.215843   14.799387   14.230846
  C      1.465231   10.971070   14.007153
  H      1.555408    9.895802   13.885846
  C      0.998069   11.546610   15.182595
  H      0.711000   10.906376   16.016740
  C      4.772299    8.396143    9.126345
  H      5.096699    9.093820    8.342809
  H      5.382595    8.555296   10.025752
  H      4.959945    7.374405    8.771509
  C      0.123191   19.820313   14.308204
  H     -0.804779   19.423897   13.875014
  H      0.402225   19.212919   15.179962
  H     -0.074453   20.840824   14.661037
  C      2.388511    8.309509    8.206694
  H      1.323979    8.405155    8.460273
  H      2.628849    9.005502    7.392033
  H      2.554803    7.287829    7.841238
  C      0.912595   20.721464   12.050004
  H      1.746786   20.749729   11.335804
  H      0.012636   20.355232   11.538378
  H      0.720821   21.750414   12.380931
  C      0.899807   12.938703   15.284630
  H      0.536421   13.420823   16.190836

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MULLIKEN ATOMIC CHARGES AND SPIN POPULATIONS
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   0 Fe:   -0.240742    0.389368
```

1	O	:	-0.326087	-0.001907
2	N	:	-0.042518	0.296830
3	N	:	-0.044029	0.297403
4	N	:	0.011862	0.043796
5	N	:	0.049848	0.171671
6	N	:	0.047159	-0.013668
7	N	:	0.050414	-0.013676
8	N	:	0.052354	0.171642
9	O	:	-0.325733	-0.001908
10	N	:	-0.026755	0.132351
11	N	:	-0.027523	0.132164
12	N	:	-0.188298	0.277322
13	N	:	0.014827	0.043773
14	N	:	-0.190735	0.277323
15	C	:	0.202095	-0.041184
16	C	:	-0.180150	0.053370
17	H	:	0.213528	-0.001681
18	C	:	0.063260	-0.105554
19	C	:	0.158606	0.017483
20	C	:	-0.051437	0.007952
21	H	:	0.178021	-0.000278
22	C	:	0.330491	-0.015782
23	C	:	0.201705	-0.041220
24	C	:	-0.119959	-0.019059
25	H	:	0.171189	0.001013
26	C	:	-0.122809	0.049171
27	H	:	0.169086	-0.002039
28	C	:	-0.188031	-0.021258
29	H	:	0.177906	0.000630
30	C	:	0.058950	-0.105543
31	C	:	-0.121887	-0.019091
32	H	:	0.169735	0.001010
33	C	:	-0.052352	0.006965
34	H	:	0.159450	-0.000158
35	C	:	0.154062	0.017250
36	C	:	-0.052791	0.006930
37	H	:	0.158774	-0.000143
38	C	:	-0.180380	-0.021224
39	H	:	0.177608	0.000630
40	C	:	-0.063767	-0.024054
41	H	:	0.178796	0.000806
42	C	:	0.022634	-0.010374
43	H	:	0.149462	0.000453
44	C	:	0.332698	-0.015761
45	C	:	-0.046906	0.007974
46	H	:	0.178506	-0.000278
47	C	:	-0.065997	-0.014455
48	H	:	0.158643	0.000440
49	C	:	0.023750	-0.010410
50	H	:	0.148888	0.000453
51	C	:	-0.061433	-0.014379
52	H	:	0.156895	0.000404
53	C	:	-0.178835	0.053379
54	H	:	0.213214	-0.001685

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  55 C :   -0.062913   -0.024042
  56 H :    0.178505    0.000801
  57 C :   -0.348889    0.009012
  58 H :    0.126416   -0.000496
  59 H :    0.122340    0.000001
  60 H :    0.151364   -0.000166
  61 C :   -0.348664    0.009037
  62 H :    0.126466   -0.000502
  63 H :    0.122040    0.000002
  64 H :    0.151461   -0.000166
  65 C :   -0.347348    0.008809
  66 H :    0.121774    0.000014
  67 H :    0.126192   -0.000496
  68 H :    0.151185   -0.000191
  69 C :   -0.348508    0.008810
  70 H :    0.122269    0.000011
  71 H :    0.126448   -0.000493
  72 H :    0.151533   -0.000197
  73 C :   -0.126865    0.049101
  74 H :    0.169930   -0.002033
Sum of atomic charges         :    2.0000000
Sum of atomic spin populations:    2.0000000
```

ABSORPTION SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS

State	Energy (cm-1)	Wavelength (nm)	fosc	T2 (au**2)	TX (au)	TY (au)	TZ (au)
1	11806.5	847.0	0.000162067	0.00452	0.01188	0.04867	0.04482
2	11936.8	837.7	0.010689926	0.29482	0.02333	-0.52454	-0.13835
3	12198.6	819.8	0.000165901	0.00448	0.01813	-0.05953	-0.02459
4	12582.6	794.7	0.000004209	0.00011	0.00057	0.00989	0.00347
5	13018.5	768.1	0.005513410	0.13942	0.02068	-0.35880	-0.10130
6	13720.0	728.9	0.131442145	3.15395	0.09342	-1.70884	-0.47445
7	15607.7	640.7	0.000631316	0.01332	0.03630	0.01929	-0.10783
8	15692.9	637.2	0.000625351	0.01312	0.10786	-0.01152	0.03677
9	17023.4	587.4	0.000119434	0.00231	0.02004	-0.01586	0.04070
10	18022.4	554.9	0.000028557	0.00052	0.02226	0.00439	-0.00266
11	18040.2	554.3	0.000014788	0.00027	0.00144	0.00392	-0.01589
12	18594.1	537.8	0.000105021	0.00186	0.03152	0.02610	-0.01359
13	18657.1	536.0	0.000072995	0.00129	0.01971	0.00316	0.02983
14	19229.9	520.0	0.023830269	0.40797	0.31308	0.55663	-0.01072
15	20376.6	490.8	0.021727206	0.35103	0.25708	-0.13786	0.51569
16	21969.9	455.2	0.080895935	1.21220	-0.67783	0.77491	0.39020
17	22011.9	454.3	0.019151139	0.28643	0.01670	0.11699	0.52198
18	22273.1	449.0	0.000807922	0.01194	-0.03096	-0.05053	0.09182
19	22327.0	447.9	0.000909695	0.01341	-0.10710	0.00169	-0.04406
20	20353.0	491.3	0.002947298	0.04767	-0.07496	0.15986	0.12844
21	20404.0	490.1	0.001366731	0.02205	0.08590	-0.12110	-0.00288
22	20973.5	476.8	0.000521026	0.00818	-0.08151	0.02843	-0.02694
23	20965.9	477.0	0.000811368	0.01274	-0.01125	0.01259	-0.11160
24	25821.1	387.3	0.009793566	0.12487	-0.16559	0.06291	-0.30576

```
  25   25767.6    388.1   0.000080788   0.00103  -0.00614   0.01141  -0.02940
  26   25799.0    387.6   0.000421379   0.00538  -0.05721  -0.04262   0.01695
  27   26108.4    383.0   0.011276327   0.14219   0.32073   0.13115  -0.14873
  28   26240.9    381.1   0.002471869   0.03101  -0.03181  -0.07822  -0.15453
  29   26308.2    380.1   0.027635463   0.34582   0.17262  -0.52918  -0.18973
  30   26931.3    371.3   0.010228250   0.12503   0.13074  -0.29646  -0.14161
  31   27025.4    370.0   0.000029629   0.00036   0.00820  -0.00510   0.01636
  32   27602.1    362.3   0.014494147   0.17287  -0.19080   0.09088  -0.35806
  33   27673.0    361.4   0.006354104   0.07559  -0.24118   0.00023   0.13201
  34   27811.5    359.6   0.000282593   0.00335   0.05464  -0.00274  -0.01876
  35   28281.5    353.6   0.030866324   0.35930   0.46680  -0.22960  -0.29780
  36   28381.8    352.3   0.008790482   0.10196  -0.15412   0.08114  -0.26763
  37   27748.8    360.4   0.005786628   0.06865   0.16269   0.20279   0.03257
  38   27462.7    364.1   0.002406453   0.02885   0.00065   0.12570  -0.11423
  39   28952.0    345.4   0.006075996   0.06909   0.04008  -0.24780  -0.07796
  40   28939.5    345.5   0.000131778   0.00150   0.00878   0.02378   0.02927
  41   29075.9    343.9   0.003656235   0.04140   0.00385   0.19948   0.03990
  42   29585.3    338.0   0.007458314   0.08299   0.12141  -0.04331   0.25764
  43   29461.6    339.4   0.004824514   0.05391  -0.09220  -0.21296   0.00762
  44   29938.9    334.0   0.001596246   0.01755  -0.04190   0.00686  -0.12550
  45   29970.5    333.7   0.000830568   0.00912   0.02794  -0.06432  -0.06485
  46   29681.8    336.9   0.035325256   0.39181   0.25081  -0.52422  -0.23257
  47   30323.1    329.8   0.002261608   0.02455   0.03069   0.15129   0.02688
  48   29989.1    333.5   0.005516647   0.06056  -0.05142   0.02390  -0.23947
  49   29700.0    336.7   0.012565058   0.13928   0.30360  -0.16151  -0.14499
  50   30521.2    327.6   0.000315745   0.00341   0.04770  -0.02812   0.01842

-----------------------------------------
BROKEN SYMMETRY MAGNETIC COUPLING ANALYSIS
-----------------------------------------

S(High-Spin)      =   1.0
<S**2>(High-Spin) =   2.0518
<S**2>(BrokenSym) =   1.0482
E(High-Spin)      = -3231.727663 Eh
E(BrokenSym)      = -3231.726555 Eh
E(High-Spin)-E(BrokenSym)= -0.0301 eV   -243.005 cm**-1 (FERROMAGNETIC coupling)

         ------------------------------------------------------
         | Spin-Hamiltonian Analysis based on H(HDvV)= -2J*SA*SB |
   -------                                                      -----------
   | J(1) =     243.01 cm**-1    (from -(E[HS]-E[BS])/Smax**2)              |
   | J(2) =     121.50 cm**-1    (from -(E[HS]-E[BS])/(Smax*(Smax+1))       |
   | J(3) =     242.13 cm**-1    (from -(E[HS]-E[BS])/(<S**2>HS-<S**2>BS)) |
   ---------------------------------------------------------------------------

  J(1): (a) A.P. Ginsberg J. Am. Chem. Soc. 102 (1980), 111
        (b) L. Noodleman J. Chem. Phys. 74 (1981), 5737
        (c) L. Noodleman E.R. Davidson Chem. Phys. 109 (1985), 131
  J(2)  (d) A. Bencini D. Gatteschi J. Am. Chem. Soc. 108 (1980), 5763
  J(3)  (e) K. Yamaguchi Y. Takahara T. Fueno in: V.H. Smith (Ed.)
            Applied Quantum Chemistry. Reidel, Dordrecht (1986), pp 155
        (f) T.Soda et al. Chem. Phys. Lett., 319, (2000), 223
```

E. $[Ni(dipyvd)_2]^{2+}$ S=2

```
  --------------------------------
CARTESIAN COORDINATES (ANGSTROEM)
--------------------------------
  Ni    15.818820    0.071317    3.841555
  N     11.262106    1.115040    3.810351
  C     13.029054   -0.093771    3.063910
  N     13.901682    0.540345    3.860991
  C     12.039151    1.869101    4.705899
  N     14.987674   -1.278766    2.380839
  C     13.647269   -1.134064    2.217074
  C     12.916288   -1.911654    1.316199
  H     11.842425   -1.755697    1.222869
  C     13.589791   -2.870001    0.559427
  H     13.045567   -3.491522   -0.151999
  C     14.967722   -3.020427    0.726889
  H     15.531100   -3.757250    0.155314
  C     15.626110   -2.204967    1.647439
  H     16.701433   -2.293614    1.807188
  N     15.670279    1.622236    5.293477
  C     14.429305    2.129868    5.492344
  C     14.179145    3.159692    6.412498
  H     13.172896    3.542467    6.545620
  C     15.254582    3.664666    7.138255
  H     15.083858    4.465012    7.858594
  C     16.536138    3.145384    6.940161
  H     17.396783    3.519108    7.492974
  C     16.693348    2.126247    6.008248
  H     17.671055    1.683712    5.815501
  C     21.784465   -1.519167    3.967195
  H     22.298017   -0.879509    3.240229
  C     22.325364   -1.248471    5.371545
  H     23.389117   -1.518108    5.398255
  H     21.800739   -1.852635    6.123395
  H     22.241891   -0.186517    5.639512
  C     21.898993   -2.983857    3.542215
  H     21.518856   -3.140678    2.523624
  H     21.358359   -3.642712    4.234598
  H     22.957989   -3.272892    3.552435
  N     20.349275   -1.080063    3.883918
  C     19.999936   -0.071751    2.969762
  C     18.227645   -1.332167    4.642963
  N     18.606924    0.252341    2.982931
  N     17.738473   -0.386790    3.826864
  N     19.493886   -1.711794    4.711607
  O     20.797661    0.473963    2.238310
  N     16.653675    1.348743    2.356863
  C     17.989009    1.229906    2.156696
  C     18.678278    2.009344    1.214804
  H     19.748006    1.888182    1.081427
```

C	17.948919	2.930752	0.468230
H	18.463401	3.547321	-0.269161
C	16.572173	3.057781	0.667542
H	15.974791	3.768831	0.098759
C	15.970590	2.245888	1.621838
H	14.899364	2.302828	1.817194
N	15.946344	-1.476625	5.336779
C	17.205412	-1.956235	5.507244
C	17.503386	-2.961853	6.429432
H	18.530193	-3.311569	6.527259
C	16.468969	-3.490062	7.201305
H	16.671640	-4.275535	7.929690
C	15.173869	-2.998362	7.026983
H	14.337922	-3.383918	7.609685
C	14.957734	-1.992658	6.084748
H	13.960194	-1.583697	5.919434
C	9.784816	1.380295	3.729418
H	9.621377	2.185725	4.454553
C	9.426073	1.865234	2.324156
H	8.356316	2.109967	2.297197
H	9.617581	1.087497	1.573065
H	9.984238	2.772135	2.054717
C	9.014270	0.130649	4.158067
H	9.278632	-0.177178	5.178855
H	9.197562	-0.705378	3.470176
H	7.939893	0.355495	4.143578
N	11.728897	0.145940	2.998747
N	13.426986	1.523346	4.687671
O	11.583178	2.730954	5.425891

ABSORPTION SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS

State	Energy (cm-1)	Wavelength (nm)	fosc	T2 (au**2)	TX (au)	TY (au)	TZ (au)
1	13752.2	727.2	0.000000166	0.00000	-0.00072	0.00078	-0.00169
2	16573.9	603.4	0.000366116	0.00727	0.03847	-0.01837	-0.07386
3	16630.7	601.3	0.000266112	0.00527	0.01700	0.07001	-0.00879
4	18825.1	531.2	0.077867129	1.36173	-0.78045	0.27795	-0.82181
5	18890.5	529.4	0.040837283	0.71169	-0.28636	-0.78927	-0.08206
6	20613.5	485.1	0.000249197	0.00398	0.01306	0.05934	-0.01698
7	21430.3	466.6	0.000359526	0.00552	0.00505	0.02461	0.06994
8	21622.1	462.5	0.000212760	0.00324	0.00583	0.03256	-0.04632
9	21321.6	469.0	0.000202717	0.00313	0.01354	0.05239	0.01421
10	22549.7	443.5	0.072176123	1.05373	-0.94574	0.24675	-0.31373
11	22588.6	442.7	0.009233912	0.13458	0.14198	0.33804	0.01203
12	23201.9	431.0	0.000007593	0.00011	0.00238	0.00979	0.00248
13	24042.5	415.9	0.000850256	0.01164	-0.00456	-0.01915	-0.10609
14	24081.4	415.3	0.000554703	0.00758	-0.01905	-0.08153	0.02394
15	24551.4	407.3	0.049621292	0.66538	0.61142	-0.14169	-0.52102
16	25254.1	396.0	0.016197494	0.21115	0.09254	0.45005	0.00619
17	25263.4	395.8	0.000016248	0.00021	-0.00696	0.00831	0.00970
18	22669.3	441.1	0.000580839	0.00844	0.08172	0.02115	0.03619

19	22962.4	435.5	0.000914763	0.01311	0.08612	-0.05467	0.05204
20	25648.2	389.9	0.000025180	0.00032	-0.01488	-0.00701	-0.00726
21	25897.3	386.1	0.005146854	0.06543	0.08908	0.18921	-0.14729
22	25946.2	385.4	0.005377614	0.06823	0.03144	-0.16306	-0.20163
23	27436.0	364.5	0.022945118	0.27533	0.48911	-0.10784	-0.15643
24	27806.3	359.6	0.009312167	0.11025	-0.06305	-0.32589	-0.00852
25	28509.9	350.8	0.000279889	0.00323	0.04975	-0.02619	0.00843
26	28531.6	350.5	0.000301803	0.00348	0.03686	0.04551	0.00724
27	27514.4	363.4	0.000017894	0.00021	-0.00732	0.00094	-0.01264
28	27584.5	362.5	0.000005453	0.00007	0.00415	-0.00422	0.00549
29	29566.3	338.2	0.110070499	1.22560	0.98179	-0.11801	0.49776
30	29741.4	336.2	0.023666312	0.26197	-0.12661	0.48007	-0.12436
31	29853.9	335.0	0.002398074	0.02644	-0.02377	-0.16057	0.00986
32	29863.2	334.9	0.000371667	0.00410	-0.05897	0.02216	-0.01133
33	30134.4	331.8	0.013370729	0.14607	-0.12065	-0.31620	0.17757
34	30166.8	331.5	0.014918042	0.16280	-0.06489	0.18449	0.35292
35	30847.5	324.2	0.004526648	0.04831	-0.01591	0.04292	-0.21498
36	30925.7	323.4	0.003664076	0.03900	0.04938	0.18922	0.02762
37	27046.5	369.7	0.000156164	0.00190	0.02223	-0.01555	-0.03413
38	27030.6	370.0	0.000218766	0.00266	-0.03188	0.00575	0.04019
39	28776.6	347.5	0.003147140	0.03600	0.10943	0.05455	0.14510
40	28832.8	346.8	0.002426537	0.02771	0.03958	-0.12302	0.10490
41	32105.2	311.5	0.066173705	0.67856	0.45800	0.60678	0.31718
42	32159.5	311.0	0.087632815	0.89708	-0.50045	0.47309	-0.65024
43	32258.6	310.0	0.014950381	0.15257	0.25602	-0.05614	0.28962
44	32542.3	307.3	0.000243286	0.00246	-0.02641	0.01812	-0.03789
45	32254.8	310.0	0.031387001	0.32036	-0.30996	-0.32430	-0.34512
46	32303.3	309.6	0.024659149	0.25131	-0.10601	0.39626	-0.28818
47	32396.4	308.7	0.027850001	0.28301	-0.10802	0.17790	-0.48959
48	32317.2	309.4	0.014383892	0.14653	-0.12414	-0.30875	-0.18919
49	32784.0	305.0	0.025846766	0.25955	-0.02731	0.20502	-0.46559
50	32761.9	305.2	0.020996040	0.21098	0.12347	0.40737	0.17258