Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Assessment of the ground spin state of iron(I) complexes : insights from DFT predictive models

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1) General considerations

All DFT computations at the OPBE level were performed using Gaussian09 version D.01[1a], except for structures which were optimized at the OPBE-D3(BJ) level, for which Gaussian09 version E.01[1b] was used, and computation of Mössbauer isomer shifts, which were performed using the ORCA software (see section 5 of this SI file). Unless specified otherwise, all structures were characterized as minima by frequency analysis (no imaginary frequency), and were optimized without geometrical constraint except for ^{2}**12**, in which Fe was forced to keep a tetrahedral environment (no tetrahedral geometry for the doublet state could be reached otherwise).

Unrestricted DFT methods were applied. OPBE functional was chosen, associated with Ahlrichs's triple-zeta basis set (def2-TZVP)[2] for iron and 6-31G* for other atoms (C, H, N, O, P, Si)[3] unless specified otherwise (several structures were computed using the def2-TZVP basis set on all atoms, and are given at the end of the section 2 of this SI file). For all the computed structures, the stability of the optimized wavefunction was checked using the *stable=opt* command implemented in Gaussian. All structures computed in this work appeared to be stable (with no internal instability).

2) DFT-computed structures

Spin multiplicities are superscripted; the structures of the computed complexes are displayed in the article, Scheme 2.

	^{4}**1**		
Fe	-0.144596000	0.025249000	-0.427838000
C	1.205882000	0.133610000	2.374237000
C	-1.362110000	0.129454000	2.423433000
C	-0.067413000	0.176727000	2.973195000
H	-0.047298000	0.233114000	4.061411000
C	-0.069385000	-1.415882000	-2.105458000
C	-1.351469000	-0.805044000	-2.165667000
C	1.087867000	-0.597966000	-2.200610000
C	-1.470412000	0.598708000	-2.195922000
H	-2.251562000	-1.412659000	-2.143468000
C	0.968387000	0.810520000	-2.190024000
H	2.075844000	-1.050548000	-2.177020000
C	-0.314761000	1.420775000	-2.123528000
H	-2.461107000	1.042517000	-2.168889000
H	1.864380000	1.425564000	-2.183807000
H	-0.406194000	2.505304000	-2.124918000
N	1.415069000	0.056037000	1.058287000
N	-1.640836000	0.068869000	1.111705000
H	0.023928000	-2.500441000	-2.092738000
C	-3.011735000	0.023690000	0.709640000
C	-3.700041000	1.235390000	0.392638000
C	-3.685707000	-1.228617000	0.582510000
C	-5.013164000	1.155986000	-0.096082000
C	-4.994688000	-1.241002000	0.075597000
C	-5.656314000	-0.066904000	-0.275699000
H	-5.548850000	2.075022000	-0.336597000
H	-5.515242000	-2.193981000	-0.029615000
H	-6.675047000	-0.102454000	-0.665795000
C	2.749247000	-0.006955000	0.561969000
C	3.364745000	-1.276667000	0.319783000
C	3.438909000	1.192009000	0.194049000
C	4.575657000	-1.307826000	-0.395870000
C	4.645575000	1.077001000	-0.520278000
C	5.208736000	-0.152794000	-0.840444000
H	5.027763000	-2.278551000	-0.612763000
H	5.152879000	1.991584000	-0.835908000
H	6.132891000	-0.210057000	-1.417738000
C	-3.081703000	2.613609000	0.625128000
H	-2.004049000	2.462409000	0.772517000
C	-3.074230000	-2.548295000	1.051964000
H	-2.050814000	-2.335308000	1.385445000
C	2.917164000	-2.673950000	0.793354000
H	3.168610000	-3.336775000	-0.053041000
C	3.081853000	2.655974000	0.524953000
H	3.353443000	3.210740000	-0.390438000

C	2.353854000	0.176363000	3.368780000
H	2.271169000	-0.657594000	4.079543000
H	3.335510000	0.124418000	2.890898000
H	2.306525000	1.100620000	3.961466000
C	-2.456747000	0.126158000	3.478742000
H	-2.316504000	0.967019000	4.171226000
H	-3.463904000	0.186179000	3.059100000
H	-2.390877000	-0.791131000	4.080163000
C	-3.847210000	-3.123624000	2.253561000
H	-3.958868000	-2.392354000	3.062245000
H	-4.856291000	-3.448977000	1.962317000
H	-3.322001000	-4.000942000	2.659888000
C	-2.982352000	-3.621252000	-0.043979000
H	-2.375425000	-3.290548000	-0.893329000
H	-2.516042000	-4.531552000	0.360898000
H	-3.972509000	-3.905756000	-0.427353000
C	-3.639743000	3.273775000	1.898963000
H	-4.717910000	3.468038000	1.801698000
H	-3.493483000	2.650567000	2.787017000
H	-3.141575000	4.238239000	2.079608000
C	-3.257552000	3.589089000	-0.550040000
H	-2.933844000	3.161830000	-1.505917000
H	-4.301956000	3.910768000	-0.668861000
H	-2.663116000	4.497015000	-0.371038000
C	4.019559000	3.189635000	1.627312000
H	3.813936000	2.710386000	2.592667000
H	5.076801000	3.015895000	1.387350000
H	3.875304000	4.273031000	1.754732000
C	1.642088000	3.069848000	0.837121000
H	0.931106000	2.690471000	0.097456000
H	1.303446000	2.736232000	1.823566000
H	1.586949000	4.169460000	0.825906000
C	3.803279000	-3.141177000	1.966098000
H	4.872532000	-3.050649000	1.733454000
H	3.608514000	-2.554425000	2.872732000
H	3.595952000	-4.196214000	2.200209000
C	1.449798000	-2.965543000	1.113594000
H	1.117185000	-2.507022000	2.050560000
H	0.777537000	-2.625446000	0.320067000
H	1.326156000	-4.054683000	1.217117000

Sum of electronic and thermal Energies= -2734.111994
Sum of electronic and thermal Enthalpies= -2734.111049
Sum of electronic and thermal Free Energies= -2734.229150
Lowest vibration frequencies (/cm^-1): 10.3939 30.5361 33.9313

^{2}1

Fe	-0.131613000	-0.007860000	-0.413731000
C	1.137742000	0.069663000	2.308109000
C	-1.391435000	0.080134000	2.300853000
C	-0.128456000	0.096184000	2.905954000
H	-0.132536000	0.132836000	3.994453000

C	-0.142786000	-1.489309000	-1.921554000
C	-1.349720000	-0.754046000	-1.958903000
C	1.074912000	-0.770010000	-1.959278000
C	-1.341702000	0.661866000	-1.999370000
H	-2.308012000	-1.258373000	-1.878894000
C	1.082823000	0.648862000	-2.002934000
H	2.022403000	-1.297136000	-1.878218000
C	-0.126137000	1.383604000	-2.007223000
H	-2.294369000	1.180394000	-1.949576000
H	2.036150000	1.169589000	-1.954513000
H	-0.118536000	2.473174000	-2.023653000
N	1.335364000	0.024355000	0.986184000
N	-1.597696000	0.036676000	0.973276000
H	-0.148350000	-2.577931000	-1.873743000
C	-2.974966000	0.024365000	0.555257000
C	-3.662789000	1.253921000	0.318456000
C	-3.661435000	-1.217492000	0.389880000
C	-4.990898000	1.204544000	-0.134442000
C	-4.989651000	-1.196446000	-0.064770000
C	-5.652060000	-0.003274000	-0.341137000
H	-5.525392000	2.137651000	-0.316597000
H	-5.522535000	-2.139243000	-0.193232000
H	-6.684262000	-0.013994000	-0.695561000
C	2.700102000	0.002196000	0.541266000
C	3.368724000	-1.244390000	0.328091000
C	3.382219000	1.226158000	0.253498000
C	4.612403000	-1.228788000	-0.331035000
C	4.626023000	1.157900000	-0.402043000
C	5.232230000	-0.049592000	-0.725734000
H	5.100888000	-2.182123000	-0.544494000
H	5.124794000	2.091152000	-0.672611000
H	6.182221000	-0.071126000	-1.262007000
C	-3.046646000	2.625380000	0.603905000
H	-1.981045000	2.469552000	0.815129000
C	-3.040521000	-2.568234000	0.751496000
H	-1.973633000	-2.397330000	0.943587000
C	2.950453000	-2.665214000	0.763935000
H	3.180444000	-3.295511000	-0.113268000
C	2.975944000	2.675263000	0.597953000
H	3.205384000	3.244638000	-0.320122000
C	2.286190000	0.098531000	3.301495000
H	2.204399000	-0.751201000	3.993439000
H	3.271238000	0.064171000	2.830997000
H	2.228436000	1.009454000	3.913413000
C	-2.528441000	0.116616000	3.309066000
H	-3.523306000	0.109898000	2.859026000
H	-2.448747000	-0.743605000	3.987414000
H	-2.436887000	1.014460000	3.935148000
C	-3.663833000	-3.147688000	2.035101000
H	-3.598846000	-2.455732000	2.880478000
H	-4.726062000	-3.389303000	1.884889000

H	-3.148826000	-4.077187000	2.320042000
C	-3.149654000	-3.629776000	-0.356199000
H	-2.730543000	-3.295360000	-1.311618000
H	-2.603932000	-4.535731000	-0.054087000
H	-4.191356000	-3.929578000	-0.538388000
C	-3.682901000	3.277827000	1.845385000
H	-4.743465000	3.509914000	1.670677000
H	-3.627018000	2.635141000	2.729579000
H	-3.170951000	4.222421000	2.082343000
C	-3.147204000	3.618312000	-0.566500000
H	-2.714412000	3.229586000	-1.494768000
H	-4.187748000	3.901221000	-0.779677000
H	-2.608914000	4.543488000	-0.313193000
C	3.913998000	3.236439000	1.687244000
H	3.747235000	2.736117000	2.649924000
H	4.973923000	3.115115000	1.429122000
H	3.722724000	4.310306000	1.831560000
C	1.531838000	3.033432000	0.955380000
H	0.808730000	2.607955000	0.254847000
H	1.250492000	2.702544000	1.960917000
H	1.431188000	4.129512000	0.932249000
C	3.879701000	-3.159561000	1.892704000
H	4.941581000	-3.055592000	1.634875000
H	3.707054000	-2.601232000	2.821939000
H	3.685612000	-4.222277000	2.101365000
C	1.502341000	-2.989461000	1.136122000
H	1.213287000	-2.578566000	2.109370000
H	0.788057000	-2.619694000	0.396284000
H	1.397345000	-4.083586000	1.198525000

Sum of electronic and thermal Energies= -2734.118884
Sum of electronic and thermal Enthalpies= -2734.117939
Sum of electronic and thermal Free Energies= -2734.229786
Lowest vibration frequencies (/cm^-1): 18.8364 29.4327 38.7286

^{4}1'

Fe	-0.003950000	-0.126077000	-0.563768000
C	1.246040000	-0.075917000	2.232766000
C	-1.251550000	-0.072468000	2.231075000
C	-0.003344000	-0.118742000	2.861047000
H	-0.004001000	-0.151033000	3.949162000
C	0.079910000	-1.699525000	-2.070418000
C	-1.183765000	-1.058054000	-2.211067000
C	1.266327000	-0.927278000	-2.218156000
C	-1.258886000	0.345659000	-2.358446000
H	-2.100099000	-1.638845000	-2.131118000
C	1.192617000	0.478982000	-2.342043000
H	2.239290000	-1.405526000	-2.130371000
C	-0.072693000	1.132632000	-2.343349000
H	-2.231354000	0.832926000	-2.376861000
H	2.107664000	1.066786000	-2.360363000
H	-0.130875000	2.216328000	-2.432781000

N	1.486596000	-0.031824000	0.922437000
N	-1.489802000	-0.027267000	0.920046000
H	0.137896000	-2.780261000	-1.948631000
H	2.120529000	-0.061579000	2.897301000
H	-2.127219000	-0.057466000	2.893908000
C	-2.868375000	0.069010000	0.571299000
C	-3.436376000	1.344697000	0.327395000
C	-3.658284000	-1.102791000	0.464073000
C	-4.780340000	1.420624000	-0.066171000
C	-4.998936000	-0.976281000	0.067723000
C	-5.559463000	0.271192000	-0.206172000
H	-5.221494000	2.401080000	-0.256913000
H	-5.611504000	-1.876005000	-0.020667000
H	-6.602091000	0.348770000	-0.517932000
C	2.866184000	0.064974000	0.578048000
C	3.653753000	-1.107414000	0.460739000
C	3.437458000	1.341424000	0.347281000
C	4.995272000	-0.980438000	0.066822000
C	4.782455000	1.418148000	-0.042433000
C	5.559297000	0.268517000	-0.192801000
H	5.605430000	-1.880909000	-0.030818000
H	5.225974000	2.399465000	-0.222830000
H	6.602578000	0.346681000	-0.502242000
C	-2.631822000	2.601683000	0.524492000
H	-2.447887000	2.792595000	1.592626000
H	-1.645000000	2.533266000	0.049069000
H	-3.157406000	3.475056000	0.117048000
C	-3.101249000	-2.458818000	0.810976000
H	-2.065283000	-2.577252000	0.470869000
H	-3.092108000	-2.617858000	1.900390000
H	-3.710756000	-3.259450000	0.371446000
C	3.090054000	-2.465893000	0.786214000
H	3.075988000	-2.641369000	1.873146000
H	2.054824000	-2.573393000	0.440587000
H	3.696921000	-3.262772000	0.336279000
C	2.636058000	2.598401000	0.556979000
H	1.646951000	2.534927000	0.085598000
H	2.457558000	2.782034000	1.627325000
H	3.161498000	3.473761000	0.153634000

Sum of electronic and thermal Energies= -2341.507308
Sum of electronic and thermal Enthalpies= -2341.506363
Sum of electronic and thermal Free Energies= -2341.596838
Lowest vibration frequencies (/cm^-1) : 12.6406 38.6255 45.7711

^{2}1'

Fe	-0.000778000	-0.104276000	-0.548556000
C	1.227106000	-0.000487000	2.140511000
C	-1.224648000	-0.007339000	2.143260000
C	0.001999000	-0.015153000	2.804055000
H	0.003263000	-0.004874000	3.891833000
C	0.037359000	-1.652683000	-1.964026000

C	-1.198087000	-0.963553000	-2.039454000
C	1.231548000	-0.893522000	-2.048017000
C	-1.237065000	0.451339000	-2.148996000
H	-2.135036000	-1.505638000	-1.926328000
C	1.193175000	0.521288000	-2.156505000
H	2.197173000	-1.383280000	-1.937963000
C	-0.042434000	1.213195000	-2.186342000
H	-2.202661000	0.952821000	-2.114642000
H	2.130296000	1.074860000	-2.131632000
H	-0.074261000	2.301594000	-2.246577000
N	1.415066000	-0.013133000	0.819151000
N	-1.414581000	-0.021730000	0.822246000
H	0.069046000	-2.736837000	-1.851354000
H	2.130517000	0.032240000	2.760600000
H	-2.127091000	0.020352000	2.764931000
C	-2.806581000	0.038520000	0.478656000
C	-3.417651000	1.301083000	0.279950000
C	-3.567298000	-1.152576000	0.395921000
C	-4.776108000	1.343491000	-0.068117000
C	-4.923632000	-1.059866000	0.043903000
C	-5.525921000	0.173955000	-0.198986000
H	-5.250829000	2.313543000	-0.229673000
H	-5.513845000	-1.975613000	-0.031660000
H	-6.579704000	0.225406000	-0.477729000
C	2.806679000	0.052573000	0.475191000
C	3.571134000	-1.136435000	0.394724000
C	3.414254000	1.316619000	0.277366000
C	4.927698000	-1.040337000	0.045624000
C	4.773098000	1.362492000	-0.069615000
C	5.526673000	0.195234000	-0.197630000
H	5.520766000	-1.954389000	-0.027328000
H	5.245480000	2.333774000	-0.230700000
H	6.580935000	0.249558000	-0.473945000
C	-2.648705000	2.579077000	0.483712000
H	-2.529324000	2.799817000	1.555787000
H	-1.637042000	2.515691000	0.065250000
H	-3.169969000	3.431210000	0.028117000
C	-2.968806000	-2.493892000	0.730512000
H	-1.906866000	-2.546287000	0.465163000
H	-3.035647000	-2.692655000	1.811897000
H	-3.504601000	-3.305065000	0.219362000
C	2.973184000	-2.478330000	0.726945000
H	3.000771000	-2.661515000	1.812763000
H	1.921872000	-2.544385000	0.424398000
H	3.534151000	-3.291198000	0.246811000
C	2.643640000	2.593291000	0.484304000
H	1.627988000	2.526666000	0.076323000
H	2.535152000	2.817183000	1.556956000
H	3.158362000	3.445287000	0.021004000

Sum of electronic and thermal Energies= -2341.521324

Sum of electronic and thermal Enthalpies= -2341.520380

Sum of electronic and thermal Free Energies= -2341.605978
Lowest vibration frequencies (/cm^-1) : 13.8576 39.9980 51.2781

^{4}**2**

Fe	0.065622000	-0.955186000	0.159139000
C	-1.367713000	-3.593600000	-0.072704000
C	1.194515000	-3.715868000	-0.170941000
C	-0.103043000	-4.219399000	0.030589000
H	-0.151187000	-5.300322000	0.157276000
N	-1.558741000	-2.271516000	-0.143121000
N	1.458869000	-2.415204000	-0.352619000
C	2.734563000	-2.016774000	-0.869943000
C	2.934257000	-2.008881000	-2.284470000
C	3.783629000	-1.591770000	-0.003624000
C	4.166576000	-1.568403000	-2.787412000
C	4.991112000	-1.156176000	-0.571355000
C	5.190645000	-1.137661000	-1.948030000
H	4.329294000	-1.564894000	-3.865579000
H	5.798244000	-0.831063000	0.085743000
H	6.139450000	-0.795484000	-2.364575000
C	-2.902756000	-1.777657000	-0.224728000
C	-3.694380000	-1.631757000	0.954420000
C	-3.430220000	-1.394878000	-1.489581000
C	-4.999423000	-1.132415000	0.823092000
C	-4.743047000	-0.904867000	-1.553626000
C	-5.530428000	-0.774873000	-0.413163000
H	-5.617105000	-1.024215000	1.715427000
H	-5.159204000	-0.623673000	-2.521626000
H	-6.550525000	-0.394182000	-0.486140000
C	1.876561000	-2.486540000	-3.275159000
H	0.952341000	-2.663542000	-2.711237000
C	3.677059000	-1.622076000	1.516461000
H	2.663461000	-1.957282000	1.768068000
C	-3.201988000	-1.995956000	2.353890000
H	-2.149333000	-2.295384000	2.270913000
C	-2.627840000	-1.509932000	-2.779813000
H	-1.613732000	-1.824371000	-2.503688000
C	2.294773000	-4.760440000	-0.174555000
H	3.239224000	-4.376531000	-0.569146000
H	2.472287000	-5.102100000	0.856087000
H	2.001162000	-5.641199000	-0.759172000
C	-2.520647000	-4.576781000	-0.169449000
H	-3.501972000	-4.101243000	-0.109760000
H	-2.459746000	-5.108583000	-1.130108000
H	-2.444676000	-5.335596000	0.620182000
C	-2.506472000	-0.160709000	-3.505812000
H	-3.478922000	0.201696000	-3.867289000
H	-2.087606000	0.613170000	-2.849640000
H	-1.848114000	-0.255888000	-4.380843000
C	-3.200184000	-2.582913000	-3.720222000
H	-4.213391000	-2.324372000	-4.059689000

H	-2.567486000	-2.686961000	-4.614195000
H	-3.255036000	-3.563615000	-3.230376000
C	1.560326000	-1.440130000	-4.355602000
H	1.277187000	-0.475170000	-3.918653000
H	2.415572000	-1.264884000	-5.022995000
H	0.727337000	-1.787615000	-4.983774000
C	2.276900000	-3.817559000	-3.934478000
H	3.180726000	-3.702742000	-4.550121000
H	2.479252000	-4.598495000	-3.191638000
H	1.470531000	-4.176977000	-4.591015000
C	3.879000000	-0.231101000	2.139210000
H	3.682632000	-0.263833000	3.220365000
H	4.908464000	0.128346000	2.002671000
H	3.206943000	0.513927000	1.694892000
C	4.653033000	-2.631216000	2.145358000
H	5.699972000	-2.339263000	1.981229000
H	4.492651000	-2.687604000	3.232233000
H	4.521511000	-3.639028000	1.732166000
C	-3.971646000	-3.183193000	2.958984000
H	-3.928940000	-4.075275000	2.323864000
H	-3.547873000	-3.447531000	3.939042000
H	-5.031638000	-2.936442000	3.114151000
C	-3.264558000	-0.803050000	3.323210000
H	-2.792998000	-1.069987000	4.280077000
H	-2.747878000	0.078139000	2.927718000
H	-4.301078000	-0.509259000	3.540155000
C	0.774871000	0.431296000	-0.907954000
C	0.355216000	-0.626191000	1.971389000
C	-1.312454000	0.560869000	0.432220000
O	1.203902000	1.313957000	-1.529196000
O	-1.580046000	1.666291000	0.676642000
O	0.434523000	-0.447877000	3.118571000

Sum of electronic and thermal Energies= -2841.895063
Sum of electronic and thermal Enthalpies= -2841.894119
Sum of electronic and thermal Free Energies= -2842.019317
Lowest vibration frequencies (/cm^-1) : 17.8951 25.5572 32.6304

^{2}2

Fe	-0.000024000	-0.951725000	-0.022638000
C	-1.339480000	-3.603439000	0.051176000
C	1.172585000	-3.671833000	-0.258574000
C	-0.076832000	-4.217229000	0.078231000
H	-0.090135000	-5.298298000	0.208588000
N	-1.522323000	-2.283058000	-0.066017000
N	1.391599000	-2.362748000	-0.431929000
C	2.699837000	-1.961986000	-0.889686000
C	2.926874000	-1.797830000	-2.285422000
C	3.754448000	-1.734526000	0.040593000
C	4.206892000	-1.419047000	-2.716907000
C	5.010300000	-1.351926000	-0.455729000
C	5.245842000	-1.196155000	-1.818321000

H	4.393943000	-1.300176000	-3.784545000
H	5.825101000	-1.175548000	0.247164000
H	6.233377000	-0.902243000	-2.177735000
C	-2.878063000	-1.806094000	-0.189128000
C	-3.659320000	-1.540581000	0.972154000
C	-3.427751000	-1.602474000	-1.486276000
C	-4.973526000	-1.079044000	0.799454000
C	-4.750871000	-1.147448000	-1.590100000
C	-5.524672000	-0.885433000	-0.463582000
H	-5.581554000	-0.870574000	1.680196000
H	-5.185389000	-0.997957000	-2.578902000
H	-6.551439000	-0.531306000	-0.569092000
C	1.846622000	-2.029664000	-3.335450000
H	0.905756000	-2.216078000	-2.802944000
C	3.594543000	-1.883789000	1.550085000
H	2.552711000	-2.162671000	1.747365000
C	-3.146331000	-1.734276000	2.395255000
H	-2.107212000	-2.078297000	2.329457000
C	-2.648228000	-1.869105000	-2.768930000
H	-1.618928000	-2.116788000	-2.480989000
C	2.260897000	-4.708105000	-0.467886000
H	3.239349000	-4.277023000	-0.687869000
H	2.346881000	-5.333312000	0.431393000
H	1.985472000	-5.376142000	-1.295260000
C	-2.500927000	-4.577751000	0.109735000
H	-3.478387000	-4.092444000	0.139672000
H	-2.474093000	-5.242605000	-0.764490000
H	-2.398405000	-5.215880000	0.998132000
C	-2.585029000	-0.629892000	-3.675378000
H	-3.577111000	-0.345497000	-4.052491000
H	-2.168909000	0.236562000	-3.146580000
H	-1.950696000	-0.831328000	-4.549987000
C	-3.208780000	-3.073434000	-3.543318000
H	-4.233211000	-2.885905000	-3.895598000
H	-2.587676000	-3.282605000	-4.427010000
H	-3.231342000	-3.979800000	-2.925456000
C	1.630433000	-0.796359000	-4.227080000
H	1.409127000	0.099021000	-3.633070000
H	2.511629000	-0.576264000	-4.845628000
H	0.788063000	-0.966988000	-4.912098000
C	2.139295000	-3.268506000	-4.198056000
H	3.057300000	-3.140099000	-4.789214000
H	2.262188000	-4.171444000	-3.587197000
H	1.313630000	-3.447770000	-4.902756000
C	3.870235000	-0.561322000	2.285579000
H	3.626047000	-0.662344000	3.352665000
H	4.928400000	-0.272837000	2.214647000
H	3.274055000	0.264065000	1.879527000
C	4.479780000	-2.999331000	2.131380000
H	5.548794000	-2.771956000	2.014321000
H	4.283703000	-3.112951000	3.207744000

H	4.292004000	-3.967917000	1.652507000
C	-3.931334000	-2.810201000	3.165169000
H	-3.938955000	-3.772816000	2.639742000
H	-3.477895000	-2.970935000	4.154372000
H	-4.976652000	-2.511947000	3.328178000
C	-3.151553000	-0.417092000	3.189654000
H	-2.662539000	-0.559428000	4.163829000
H	-2.621422000	0.382313000	2.659385000
H	-4.175177000	-0.066287000	3.382304000
C	1.127617000	0.320220000	-0.466989000
C	0.230818000	-0.754310000	1.745007000
C	-1.135915000	0.380223000	-0.167222000
O	1.783277000	1.257011000	-0.701787000
O	-1.780411000	1.351641000	-0.226210000
O	0.379239000	-0.460345000	2.863489000

Sum of electronic and thermal Energies= -2841.951530
Sum of electronic and thermal Enthalpies= -2841.950586
Sum of electronic and thermal Free Energies= -2842.068535
Lowest vibration frequencies (/cm^-1) : 18.0652 34.8484 40.9354

^{4}2'

Fe	0.042533000	-0.859341000	-0.430731000
C	-1.273883000	-3.574972000	-0.047059000
C	1.174648000	-3.693557000	-0.489645000
C	-0.062607000	-4.265140000	-0.171626000
H	-0.094955000	-5.345686000	-0.044930000
N	-1.482824000	-2.264407000	-0.165847000
N	1.402906000	-2.400693000	-0.670268000
H	-2.157739000	-4.192754000	0.160092000
H	2.026658000	-4.375647000	-0.609468000
C	2.720760000	-2.007134000	-1.048246000
C	3.047269000	-1.901809000	-2.426358000
C	3.684111000	-1.698166000	-0.053199000
C	4.309045000	-1.403753000	-2.780025000
C	4.933815000	-1.207531000	-0.461440000
C	5.243471000	-1.041050000	-1.810009000
H	4.560884000	-1.308567000	-3.838137000
H	5.676213000	-0.959030000	0.299799000
H	6.216451000	-0.645498000	-2.105549000
C	-2.852639000	-1.877019000	-0.019479000
C	-3.380472000	-1.629366000	1.271185000
C	-3.663218000	-1.747272000	-1.173650000
C	-4.720609000	-1.228256000	1.379893000
C	-4.996948000	-1.344326000	-1.011904000
C	-5.526362000	-1.081326000	0.251371000
H	-5.133684000	-1.030867000	2.370928000
H	-5.628198000	-1.240585000	-1.896597000
H	-6.565418000	-0.765367000	0.355882000
C	2.112683000	-2.377936000	-3.508310000
H	1.063095000	-2.357785000	-3.199194000
H	2.219762000	-1.772226000	-4.417756000

H	2.344943000	-3.419403000	-3.782608000
C	3.443965000	-1.946997000	1.413904000
H	2.387520000	-2.102430000	1.649469000
H	3.985392000	-2.849417000	1.739163000
H	3.815465000	-1.112672000	2.024175000
C	-2.541916000	-1.804017000	2.508816000
H	-2.307014000	-2.862310000	2.696778000
H	-1.580430000	-1.281084000	2.426032000
H	-3.065712000	-1.419578000	3.393090000
C	-3.125249000	-2.052367000	-2.545536000
H	-2.237188000	-1.449177000	-2.776629000
H	-2.820923000	-3.104930000	-2.638828000
H	-3.881555000	-1.852736000	-3.315116000
C	0.727948000	0.130681000	1.009584000
C	0.244595000	0.123278000	-2.018589000
C	-1.452657000	0.594605000	-0.200648000
O	1.117758000	0.777531000	1.892844000
O	0.362179000	0.762438000	-2.981979000
O	-1.800827000	1.701479000	-0.152798000

Sum of electronic and thermal Energies= -2449.258120
Sum of electronic and thermal Enthalpies= -2449.257176
Sum of electronic and thermal Free Energies= -2449.354892
Lowest vibration frequencies (/cm^-1) : 11.9495 26.3671 39.6741

^{2}2'

Fe	-0.132582000	-0.878131000	-0.970545000
C	-1.357467000	-3.552845000	-0.591492000
C	1.066177000	-3.589439000	-1.000713000
C	-0.176335000	-4.221354000	-0.920001000
H	-0.203350000	-5.306812000	-0.982938000
N	-1.518652000	-2.238750000	-0.478612000
N	1.294670000	-2.281154000	-0.952780000
H	-2.236383000	-4.168927000	-0.367294000
H	1.951316000	-4.232317000	-1.075358000
C	2.690459000	-1.935532000	-0.925203000
C	3.427969000	-1.839409000	-2.129449000
C	3.313987000	-1.727113000	0.330288000
C	4.788650000	-1.500820000	-2.049113000
C	4.673893000	-1.388366000	0.353713000
C	5.410173000	-1.268337000	-0.824547000
H	5.365210000	-1.422894000	-2.972813000
H	5.160457000	-1.225572000	1.317101000
H	6.468299000	-1.005274000	-0.786869000
C	-2.816172000	-1.849470000	0.003418000
C	-2.984153000	-1.632661000	1.393697000
C	-3.904324000	-1.717013000	-0.891642000
C	-4.247490000	-1.248366000	1.863519000
C	-5.150212000	-1.334659000	-0.367873000
C	-5.325787000	-1.093541000	0.992779000
H	-4.383539000	-1.076844000	2.932816000
H	-5.995802000	-1.228123000	-1.050014000

H	-6.302724000	-0.795121000	1.375907000
C	2.810184000	-2.065749000	-3.484617000
H	2.009673000	-2.813390000	-3.468129000
H	2.376083000	-1.136763000	-3.882398000
H	3.570921000	-2.399638000	-4.202350000
C	2.555151000	-1.871688000	1.621844000
H	1.744571000	-1.133659000	1.700405000
H	2.089230000	-2.862261000	1.715807000
H	3.221991000	-1.729833000	2.481470000
C	-1.846501000	-1.822066000	2.359956000
H	-1.484279000	-2.860178000	2.364626000
H	-0.985679000	-1.191235000	2.100449000
H	-2.157065000	-1.570295000	3.381668000
C	-3.775222000	-1.948046000	-2.374523000
H	-3.466963000	-1.028513000	-2.893202000
H	-3.038559000	-2.719721000	-2.623227000
H	-4.740407000	-2.250820000	-2.801270000
C	1.074298000	0.400954000	-0.904372000
C	-0.429768000	-0.705821000	-2.734012000
C	-1.211519000	0.435043000	-0.512787000
O	1.786230000	1.324527000	-0.896494000
O	-0.614751000	-0.434803000	-3.852380000
O	-1.852864000	1.378627000	-0.271597000

Sum of electronic and thermal Energies= -2449.314865
Sum of electronic and thermal Enthalpies= -2449.313921
Sum of electronic and thermal Free Energies= -2449.406637
Lowest vibration frequencies (/cm^-1) : 17.3574 25.9189 40.4935

^{4}3 (computed at the OPBE-d3bj level)

Fe	0.005365000	-0.071660000	0.007314000
C	-2.597571000	-1.371644000	-1.556247000
P	0.854638000	0.278374000	2.013574000
C	-2.791660000	-1.928210000	-0.289133000
H	-1.947999000	-1.959836000	0.387978000
P	-1.000711000	-0.580765000	-1.897240000
C	-4.046018000	-2.402522000	0.095892000
H	-4.188909000	-2.782133000	1.105273000
P	0.602421000	1.775571000	-1.165727000
C	-5.110873000	-2.338031000	-0.803411000
H	-6.098188000	-2.690781000	-0.505603000
P	-1.781417000	0.933890000	0.913049000
C	-3.662221000	-1.333446000	-2.466350000
H	-3.513107000	-0.906889000	-3.455841000
C	-0.309638000	-1.668004000	-3.163694000
C	0.060668000	-1.212391000	-4.442616000
H	-0.135333000	-0.183343000	-4.736788000
C	0.707723000	-2.065228000	-5.336019000
H	0.992132000	-1.695029000	-6.321371000
C	0.986954000	-3.385806000	-4.973799000
H	1.496159000	-4.049378000	-5.672224000
C	0.604007000	-3.849118000	-3.709872000

H	0.819613000	-4.874654000	-3.412420000
C	-0.034676000	-3.003356000	-2.810706000
H	-0.304499000	-3.361560000	-1.820755000
C	-3.006744000	1.820119000	-0.069703000
C	-2.721363000	3.117115000	-0.525426000
H	-1.846888000	3.642292000	-0.155559000
C	-3.536187000	3.722225000	-1.479656000
H	-3.299851000	4.727818000	-1.828126000
C	-4.649101000	3.045074000	-1.987380000
H	-5.279070000	3.514508000	-2.742390000
C	-4.948432000	1.762185000	-1.518811000
H	-5.809812000	1.221188000	-1.907673000
C	-4.135946000	1.148453000	-0.568962000
H	-4.359685000	0.143564000	-0.224734000
C	-2.770838000	-0.021494000	2.089788000
C	-2.197627000	-1.163265000	2.667001000
H	-1.189204000	-1.445968000	2.378632000
C	-2.903290000	-1.931484000	3.586147000
H	-2.427100000	-2.807452000	4.024270000
C	-4.209586000	-1.571148000	3.938836000
H	-4.773466000	-2.173795000	4.650163000
C	-4.784417000	-0.424910000	3.376896000
H	-5.796890000	-0.132073000	3.656260000
C	-4.070519000	0.355406000	2.469949000
H	-4.518247000	1.249906000	2.041962000
C	0.390600000	5.849530000	-0.385061000
H	-0.061193000	6.744422000	-0.813110000
C	1.150477000	5.940732000	0.786709000
H	1.285483000	6.903128000	1.279065000
C	1.737293000	4.787302000	1.312376000
H	2.342794000	4.835232000	2.217184000
C	1.545002000	3.558282000	0.688048000
H	1.990541000	2.659844000	1.102219000
C	0.780069000	3.453412000	-0.490600000
C	0.217119000	4.622182000	-1.024235000
H	-0.362760000	4.588954000	-1.942271000
C	2.248243000	1.552291000	-1.912608000
C	3.359225000	2.356771000	-1.627825000
H	3.268079000	3.177669000	-0.922745000
C	4.581504000	2.105750000	-2.247334000
H	5.436256000	2.740513000	-2.014401000
C	4.719501000	1.045724000	-3.152355000
H	5.680409000	0.851743000	-3.628304000
C	3.612551000	0.248079000	-3.447167000
H	3.691982000	-0.579461000	-4.151704000
C	2.384973000	0.500833000	-2.836922000
H	1.531592000	-0.128448000	-3.070241000
C	0.785175000	-1.874496000	-0.019823000
C	0.341496000	-3.012721000	0.670319000
H	-0.529245000	-2.970532000	1.321294000
C	1.001735000	-4.240375000	0.575607000

H	0.615404000	-5.098385000	1.128663000
C	2.168821000	-4.381842000	-0.180188000
C	2.636893000	-3.248016000	-0.858254000
H	3.534715000	-3.321752000	-1.475299000
C	1.944095000	-2.042184000	-0.798543000
H	2.305423000	-1.214967000	-1.406493000
C	2.890358000	-5.693175000	-0.278758000
H	2.401478000	-6.464595000	0.329225000
H	3.932243000	-5.602846000	0.061794000
H	2.922897000	-6.053176000	-1.317786000
C	3.393914000	0.544767000	0.944192000
H	2.963303000	0.012907000	0.103843000
C	4.734896000	0.929682000	0.930918000
H	5.347720000	0.690222000	0.065122000
C	5.268518000	1.640658000	2.004540000
H	6.311167000	1.957519000	1.988055000
C	4.465218000	1.936566000	3.113425000
H	4.886054000	2.471747000	3.964942000
C	3.135239000	1.525012000	3.143677000
H	2.526958000	1.716039000	4.025808000
C	2.584984000	0.847614000	2.045430000
C	1.094200000	-1.101649000	3.177983000
C	0.366555000	-1.303445000	4.360590000
H	-0.394463000	-0.594499000	4.672821000
C	0.590205000	-2.436429000	5.143923000
H	0.013485000	-2.575553000	6.058635000
C	1.543669000	-3.382403000	4.762550000
H	1.712566000	-4.268293000	5.374376000
C	2.278981000	-3.182799000	3.589859000
H	3.015816000	-3.917833000	3.269366000
C	2.057852000	-2.057855000	2.803973000
H	2.618286000	-1.921405000	1.882919000
C	-1.516885000	0.929151000	-2.795139000
H	-1.792981000	0.720523000	-3.833652000
H	-2.413909000	1.263409000	-2.270724000
C	-0.431678000	1.982032000	-2.699287000
H	-0.882968000	2.976132000	-2.714349000
H	0.271103000	1.914012000	-3.536909000
C	-1.089541000	2.233369000	2.021100000
H	-0.573672000	2.973721000	1.406053000
H	-1.908284000	2.719627000	2.565412000
C	-0.106279000	1.554166000	2.954690000
H	-0.658078000	1.045116000	3.749962000
H	0.571980000	2.283487000	3.408852000
C	-4.913434000	-1.819400000	-2.090632000
H	-5.744696000	-1.778026000	-2.794459000

Sum of electronic and thermal Energies= -4909.595685
Sum of electronic and thermal Enthalpies= -4909.594740
Sum of electronic and thermal Free Energies= -4909.751045
Lowest vibration frequencies (/cm^-1) : 20.7359 22.5486 29.0542

^{2}**3** (computed at the OPBE-d3bj level)

Fe	-0.067587000	-0.070272000	0.055717000
C	-2.713338000	-1.430806000	-1.505817000
P	0.824533000	0.251477000	1.968201000
C	-2.957201000	-2.065847000	-0.286833000
H	-2.136658000	-2.142543000	0.415956000
P	-1.088702000	-0.633983000	-1.730000000
C	-4.232639000	-2.527331000	0.033351000
H	-4.415487000	-2.969586000	1.010817000
P	0.599626000	1.622055000	-1.077199000
C	-5.272502000	-2.372315000	-0.886198000
H	-6.278592000	-2.708136000	-0.635213000
P	-1.722011000	0.929688000	0.897018000
C	-3.747130000	-1.317311000	-2.443820000
H	-3.562517000	-0.835018000	-3.400795000
C	-0.350849000	-1.766913000	-2.959605000
C	0.029295000	-1.356386000	-4.244047000
H	-0.141188000	-0.331866000	-4.567168000
C	0.668814000	-2.243595000	-5.112187000
H	0.967084000	-1.905627000	-6.104852000
C	0.926070000	-3.554586000	-4.708404000
H	1.433698000	-4.244536000	-5.382527000
C	0.529534000	-3.975722000	-3.437157000
H	0.732642000	-4.992588000	-3.105004000
C	-0.105154000	-3.091055000	-2.570457000
H	-0.381366000	-3.413401000	-1.571536000
C	-2.953450000	1.837017000	-0.073144000
C	-2.654209000	3.129142000	-0.528918000
H	-1.745901000	3.624019000	-0.195874000
C	-3.490482000	3.760237000	-1.448332000
H	-3.241999000	4.760403000	-1.803892000
C	-4.635043000	3.110659000	-1.919744000
H	-5.281211000	3.601019000	-2.647576000
C	-4.947101000	1.831294000	-1.452508000
H	-5.831809000	1.311888000	-1.818095000
C	-4.114501000	1.195294000	-0.533466000
H	-4.343015000	0.189640000	-0.193632000
C	-2.797829000	-0.017080000	2.045251000
C	-2.270317000	-1.179918000	2.608911000
H	-1.279331000	-1.495920000	2.291569000
C	-2.986961000	-1.913062000	3.552591000
H	-2.546875000	-2.811842000	3.982969000
C	-4.258826000	-1.484166000	3.938257000
H	-4.834566000	-2.057645000	4.664758000
C	-4.787652000	-0.307800000	3.397257000
H	-5.774617000	0.037422000	3.706296000
C	-4.056205000	0.430754000	2.466705000
H	-4.465346000	1.350513000	2.052860000
C	0.826494000	5.757909000	-0.741379000
H	0.627977000	6.629106000	-1.366138000
C	1.344819000	5.924336000	0.545042000

H	1.542633000	6.923677000	0.932041000
C	1.625744000	4.797717000	1.319570000
H	2.058614000	4.902483000	2.314216000
C	1.354890000	3.525119000	0.820161000
H	1.594114000	2.651447000	1.413618000
C	0.810921000	3.341549000	-0.456202000
C	0.580026000	4.479533000	-1.243649000
H	0.228293000	4.375977000	-2.266379000
C	2.212957000	1.560655000	-1.972120000
C	3.279684000	2.437502000	-1.739092000
H	3.176471000	3.229928000	-1.003351000
C	4.479547000	2.286854000	-2.436709000
H	5.301993000	2.975632000	-2.241138000
C	4.632812000	1.263785000	-3.374941000
H	5.573076000	1.149775000	-3.914323000
C	3.571447000	0.386423000	-3.613623000
H	3.671331000	-0.424757000	-4.334814000
C	2.376416000	0.535317000	-2.913871000
H	1.565774000	-0.167604000	-3.077321000
C	0.988711000	-1.708049000	-0.058131000
C	0.515506000	-2.852897000	0.616191000
H	-0.351055000	-2.782672000	1.269084000
C	1.129857000	-4.101240000	0.503610000
H	0.716190000	-4.952962000	1.046491000
C	2.286877000	-4.269388000	-0.262876000
C	2.792823000	-3.136367000	-0.913269000
H	3.695214000	-3.226056000	-1.521783000
C	2.151766000	-1.902634000	-0.821868000
H	2.570124000	-1.069457000	-1.377025000
C	2.962139000	-5.602497000	-0.391190000
H	2.464254000	-6.362909000	0.223663000
H	4.015332000	-5.550824000	-0.078571000
H	2.954802000	-5.954581000	-1.433589000
C	3.348283000	0.737576000	0.911725000
H	2.894430000	0.346831000	0.009536000
C	4.680708000	1.147504000	0.942466000
H	5.283389000	1.071519000	0.039918000
C	5.220413000	1.670160000	2.118364000
H	6.257720000	2.004237000	2.143300000
C	4.432640000	1.755831000	3.272027000
H	4.859042000	2.147097000	4.196060000
C	3.107972000	1.323905000	3.247150000
H	2.506216000	1.345280000	4.154480000
C	2.556166000	0.836224000	2.054566000
C	1.101864000	-1.153033000	3.122352000
C	0.336663000	-1.426566000	4.260832000
H	-0.488054000	-0.779833000	4.545043000
C	0.597490000	-2.555448000	5.040597000
H	-0.010952000	-2.749689000	5.924160000
C	1.632041000	-3.424732000	4.692510000
H	1.833207000	-4.307905000	5.298922000

C	2.407997000	-3.153836000	3.563500000
H	3.210331000	-3.829747000	3.270993000
C	2.147470000	-2.030063000	2.784690000
H	2.743597000	-1.833291000	1.897518000
C	-1.549206000	0.842531000	-2.714116000
H	-1.758029000	0.586116000	-3.757111000
H	-2.484923000	1.183623000	-2.268015000
C	-0.488056000	1.911675000	-2.581343000
H	-0.978566000	2.881584000	-2.477928000
H	0.170436000	1.946916000	-3.455093000
C	-1.158876000	2.181656000	2.129016000
H	-0.703820000	3.006832000	1.577717000
H	-2.008760000	2.556158000	2.711429000
C	-0.133168000	1.481647000	2.996837000
H	-0.652359000	0.922273000	3.779271000
H	0.551974000	2.185786000	3.480924000
C	-5.022848000	-1.785024000	-2.131266000
H	-5.832513000	-1.673667000	-2.852759000

Sum of electronic and thermal Energies= -4909.653566
Sum of electronic and thermal Enthalpies= -4909.652622
Sum of electronic and thermal Free Energies= -4909.805973
Lowest vibration frequencies (/cm^-1) : 23.4377 24.0750 29.6239

$^{4}\mathbf{3}_{\mathbf{Td}}$ (optimized at the OPBE level, without dispersion)

Fe	0.577794000	-0.255872000	1.214858000
C	-3.722052000	-1.129405000	-3.985059000
P	1.736329000	0.774864000	2.999912000
C	-4.541265000	-2.076782000	-4.633098000
H	-4.123738000	-3.047816000	-4.906829000
P	-1.983553000	-1.664061000	-3.662065000
C	-5.877257000	-1.797231000	-4.925926000
H	-6.488661000	-2.546302000	-5.432417000
P	1.046833000	0.425371000	-0.934643000
C	-6.433093000	-0.567147000	-4.559023000
H	-7.479194000	-0.348149000	-4.779933000
P	-1.372805000	0.600339000	2.124809000
C	-4.297902000	0.098958000	-3.614753000
H	-3.709144000	0.852857000	-3.094834000
C	-1.150219000	-1.206708000	-5.254860000
C	-1.514454000	-0.112757000	-6.061272000
H	-2.351487000	0.521681000	-5.769031000
C	-0.824746000	0.162483000	-7.245457000
H	-1.125744000	1.012262000	-7.861510000
C	0.244290000	-0.647516000	-7.644340000
H	0.780296000	-0.431615000	-8.570219000
C	0.613846000	-1.740926000	-6.856584000
H	1.440802000	-2.383836000	-7.163404000
C	-0.083871000	-2.022553000	-5.677464000
H	0.198806000	-2.888714000	-5.076373000
C	-2.850668000	1.340197000	1.279338000
C	-2.884792000	2.683940000	0.862508000

H	-2.037727000	3.342123000	1.045784000
C	-4.003443000	3.203692000	0.204741000
H	-4.008828000	4.253265000	-0.095491000
C	-5.108182000	2.390315000	-0.062640000
H	-5.984819000	2.799648000	-0.567289000
C	-5.075866000	1.044953000	0.318292000
H	-5.924914000	0.393610000	0.104671000
C	-3.959757000	0.524958000	0.977466000
H	-3.961898000	-0.523022000	1.278050000
C	-2.233231000	-0.434431000	3.411484000
C	-1.869892000	-1.780262000	3.576207000
H	-1.102783000	-2.208715000	2.932294000
C	-2.486792000	-2.571642000	4.552866000
H	-2.194908000	-3.618082000	4.657877000
C	-3.469946000	-2.027532000	5.382476000
H	-3.949347000	-2.643331000	6.145560000
C	-3.843395000	-0.687784000	5.224739000
H	-4.617094000	-0.255652000	5.862323000
C	-3.235486000	0.100304000	4.244894000
H	-3.561752000	1.133366000	4.118609000
C	0.470129000	3.842265000	-3.281297000
H	0.336832000	4.083067000	-4.337732000
C	0.484325000	4.862529000	-2.325178000
H	0.359221000	5.903032000	-2.629995000
C	0.667415000	4.538973000	-0.977694000
H	0.695640000	5.327007000	-0.222669000
C	0.816160000	3.203208000	-0.592280000
H	0.961182000	2.952975000	0.457769000
C	0.804875000	2.166000000	-1.538803000
C	0.638993000	2.508976000	-2.894702000
H	0.656064000	1.739827000	-3.665772000
C	2.793776000	0.093383000	-1.504528000
C	3.640591000	1.087298000	-2.028384000
H	3.286241000	2.112328000	-2.124163000
C	4.942326000	0.776862000	-2.437275000
H	5.578237000	1.565249000	-2.845601000
C	5.424576000	-0.530653000	-2.335074000
H	6.438977000	-0.771167000	-2.658016000
C	4.593564000	-1.526136000	-1.812345000
H	4.954878000	-2.552150000	-1.721184000
C	3.295224000	-1.218768000	-1.397067000
H	2.673323000	-2.005689000	-0.974632000
C	0.734532000	-2.248587000	1.056530000
C	-0.290230000	-3.055084000	0.498641000
H	-1.210086000	-2.588202000	0.133395000
C	-0.196925000	-4.447334000	0.397728000
H	-1.024305000	-5.010742000	-0.043968000
C	0.940706000	-5.134249000	0.855811000
C	1.969752000	-4.361940000	1.415975000
H	2.869058000	-4.859657000	1.791207000
C	1.867019000	-2.967554000	1.508923000

H	2.707225000	-2.430100000	1.954186000
C	1.050649000	-6.632137000	0.732193000
H	0.130656000	-7.136007000	1.064493000
H	1.883543000	-7.027736000	1.329227000
H	1.221405000	-6.938534000	-0.312700000
C	3.765411000	2.163029000	1.656216000
H	3.631857000	1.377853000	0.913787000
C	4.737200000	3.148476000	1.455164000
H	5.357407000	3.115427000	0.558413000
C	4.903415000	4.171410000	2.392421000
H	5.652473000	4.948941000	2.232918000
C	4.105559000	4.189015000	3.540735000
H	4.234845000	4.976600000	4.285641000
C	3.149725000	3.191118000	3.750928000
H	2.575878000	3.211074000	4.676799000
C	2.955112000	2.167688000	2.804290000
C	2.632734000	-0.296899000	4.222362000
C	1.924745000	-1.297260000	4.915419000
H	0.858256000	-1.434093000	4.745385000
C	2.576897000	-2.142605000	5.815424000
H	2.003723000	-2.905808000	6.344638000
C	3.953552000	-2.022620000	6.027935000
H	4.462992000	-2.686911000	6.727887000
C	4.671046000	-1.049752000	5.327765000
H	5.747549000	-0.947841000	5.477198000
C	4.019245000	-0.194148000	4.434256000
H	4.599263000	0.560290000	3.905745000
C	-1.303925000	-0.363363000	-2.490491000
H	-1.475589000	0.653217000	-2.866810000
H	-1.867804000	-0.468967000	-1.553630000
C	0.185639000	-0.608300000	-2.255493000
H	0.747843000	-0.491214000	-3.191483000
H	0.348358000	-1.642045000	-1.921704000
C	-0.772801000	2.013152000	3.199386000
H	-0.441825000	2.835096000	2.551048000
H	-1.589740000	2.396484000	3.827587000
C	0.384104000	1.517696000	4.060722000
H	0.033694000	0.717300000	4.726000000
H	0.758295000	2.321261000	4.708220000
C	-5.640314000	0.374761000	-3.898988000
H	-6.065037000	1.335667000	-3.602861000

Sum of electronic and thermal Energies= -4908.616562
Sum of electronic and thermal Enthalpies= -4908.615618
Sum of electronic and thermal Free Energies= -4908.785205
Lowest vibration frequencies (/cm^-1) : -17.1898(*) 12.0039 15.9904
(*) rotation of one phenyl ligand

^{2}**3** (optimized at the OPBE level, without dispersion)

Fe	-0.016085000	-0.130343000	0.032540000
C	-2.750800000	-1.597478000	-1.895448000
P	1.007227000	0.213882000	2.004291000

C	-3.199782000	-2.308428000	-0.774208000
H	-2.598394000	-2.306234000	0.128625000
P	-1.096842000	-0.725357000	-1.859881000
C	-4.411686000	-3.007652000	-0.794361000
H	-4.735614000	-3.549513000	0.095819000
P	0.807450000	1.598361000	-1.253701000
C	-5.202488000	-3.003948000	-1.944926000
H	-6.150175000	-3.544816000	-1.965404000
P	-1.698068000	0.994616000	1.000164000
C	-3.548475000	-1.619919000	-3.055676000
H	-3.218089000	-1.115476000	-3.962636000
C	-0.346546000	-1.776644000	-3.219174000
C	-0.158844000	-1.327691000	-4.539887000
H	-0.392928000	-0.303372000	-4.822276000
C	0.328674000	-2.183522000	-5.534174000
H	0.465426000	-1.802924000	-6.548284000
C	0.631737000	-3.513038000	-5.233846000
H	1.009712000	-4.181513000	-6.009374000
C	0.441216000	-3.976168000	-3.929256000
H	0.671144000	-5.012091000	-3.674918000
C	-0.040537000	-3.120896000	-2.936010000
H	-0.176811000	-3.505760000	-1.929047000
C	-3.062854000	2.003082000	0.213707000
C	-3.026364000	3.406748000	0.128073000
H	-2.184695000	3.963284000	0.531198000
C	-4.071325000	4.122017000	-0.468544000
H	-4.017688000	5.211768000	-0.510707000
C	-5.177444000	3.452690000	-0.997301000
H	-5.992089000	4.011588000	-1.460965000
C	-5.230744000	2.057520000	-0.917306000
H	-6.089489000	1.515701000	-1.317840000
C	-4.190816000	1.344173000	-0.316982000
H	-4.266083000	0.261212000	-0.251526000
C	-2.800081000	0.118303000	2.250935000
C	-2.562931000	-1.213012000	2.615089000
H	-1.722754000	-1.740274000	2.170080000
C	-3.361338000	-1.865115000	3.562691000
H	-3.149443000	-2.903778000	3.822423000
C	-4.412623000	-1.184043000	4.178492000
H	-5.040018000	-1.687450000	4.916206000
C	-4.650951000	0.154304000	3.845061000
H	-5.465175000	0.701535000	4.324188000
C	-3.856600000	0.795932000	2.892082000
H	-4.074103000	1.832926000	2.635938000
C	0.187463000	5.739612000	-0.747018000
H	-0.425747000	6.521549000	-1.199584000
C	1.064675000	6.050914000	0.293878000
H	1.146154000	7.074636000	0.662738000
C	1.835286000	5.028365000	0.855452000
H	2.530358000	5.244965000	1.668881000
C	1.725773000	3.718985000	0.379364000

H	2.342308000	2.946526000	0.832203000
C	0.854882000	3.383938000	-0.679153000
C	0.086352000	4.428013000	-1.226060000
H	-0.621881000	4.240246000	-2.029668000
C	2.475074000	1.592973000	-2.155976000
C	3.387556000	2.662249000	-2.177838000
H	3.178490000	3.575521000	-1.625720000
C	4.572167000	2.587563000	-2.920425000
H	5.257484000	3.437767000	-2.917808000
C	4.872568000	1.446787000	-3.667838000
H	5.795294000	1.391978000	-4.248125000
C	3.969441000	0.379523000	-3.668810000
H	4.176638000	-0.519139000	-4.252891000
C	2.790824000	0.453369000	-2.921621000
H	2.103870000	-0.390788000	-2.942082000
C	1.034858000	-1.852193000	-0.034790000
C	0.426796000	-3.001068000	0.534103000
H	-0.551011000	-2.925090000	1.009412000
C	1.013886000	-4.270917000	0.529328000
H	0.475622000	-5.105193000	0.989041000
C	2.279083000	-4.490232000	-0.038531000
C	2.911466000	-3.369659000	-0.593320000
H	3.902191000	-3.479935000	-1.044334000
C	2.306797000	-2.104933000	-0.592385000
H	2.868672000	-1.296929000	-1.053267000
C	2.909210000	-5.858861000	-0.063354000
H	2.801801000	-6.374984000	0.902408000
H	3.981602000	-5.805231000	-0.296035000
H	2.443449000	-6.506817000	-0.824150000
C	3.693299000	0.727699000	1.124769000
H	3.342381000	0.420212000	0.146212000
C	5.031787000	1.103078000	1.295645000
H	5.709431000	1.071925000	0.441203000
C	5.490107000	1.520164000	2.546173000
H	6.531566000	1.817380000	2.681347000
C	4.603691000	1.546260000	3.629280000
H	4.951595000	1.859092000	4.615690000
C	3.273493000	1.157859000	3.459072000
H	2.613781000	1.146721000	4.327050000
C	2.793171000	0.755045000	2.196694000
C	1.153056000	-1.160082000	3.282162000
C	0.291221000	-1.316231000	4.380556000
H	-0.563748000	-0.660157000	4.523397000
C	0.492219000	-2.331515000	5.323041000
H	-0.192661000	-2.418008000	6.168859000
C	1.558335000	-3.221588000	5.185637000
H	1.719013000	-4.010180000	5.922951000
C	2.416136000	-3.089731000	4.089833000
H	3.250437000	-3.780623000	3.957606000
C	2.216081000	-2.075170000	3.152070000
H	2.897389000	-1.997075000	2.307935000

C	-1.479550000	0.860511000	-2.747010000
H	-1.920484000	0.701144000	-3.740584000
H	-2.235368000	1.365119000	-2.136886000
C	-0.210204000	1.688372000	-2.841815000
H	-0.428254000	2.723090000	-3.130859000
H	0.447013000	1.296844000	-3.626253000
C	-0.944631000	2.248327000	2.156836000
H	-0.493614000	3.024543000	1.532295000
H	-1.708742000	2.714080000	2.795164000
C	0.130169000	1.572333000	2.990173000
H	-0.313746000	1.133989000	3.889474000
H	0.874144000	2.305095000	3.327192000
C	-4.764520000	-2.306225000	-3.076236000
H	-5.368635000	-2.303372000	-3.985554000

Sum of electronic and thermal Energies= -4908.604430
Sum of electronic and thermal Enthalpies= -4908.603486
Sum of electronic and thermal Free Energies= -4908.765328
Lowest vibration frequencies (/cm^-1) : 6.4312 20.1538 26.5133

$^{4}4_{Me}$

C	3.871204000	-1.658427000	0.366198000
C	2.791465000	-0.787468000	0.575996000
C	1.690713000	-0.693297000	-0.308746000
C	1.751627000	-1.560819000	-1.426538000
C	2.820275000	-2.436083000	-1.658384000
C	3.892958000	-2.489418000	-0.759227000
H	4.698108000	-1.692309000	1.084132000
H	2.815355000	-0.158410000	1.474044000
H	0.923727000	-1.561797000	-2.144042000
H	2.817032000	-3.086335000	-2.539788000
H	4.729264000	-3.173150000	-0.929925000
Fe	0.094735000	0.583411000	-0.077675000
C	0.773664000	2.326859000	-0.889178000
C	-0.587663000	2.217458000	-1.373569000
C	0.899162000	2.414045000	0.531422000
C	-1.665234000	2.759733000	-0.581492000
C	-0.256893000	2.465802000	1.361967000
H	1.892242000	2.377071000	0.985351000
C	-1.512073000	2.852003000	0.786126000
H	-2.625700000	2.981063000	-1.052634000
H	-0.128322000	2.460380000	2.445182000
H	-2.345414000	3.137425000	1.431216000
H	-0.731316000	2.102331000	-2.450326000
C	-1.545202000	-0.591961000	0.106732000
C	-2.771011000	-0.503580000	-0.596706000
C	-1.470633000	-1.674507000	1.022272000
C	-3.833905000	-1.398455000	-0.404089000
H	-2.908455000	0.300232000	-1.324511000
C	-2.524205000	-2.571961000	1.238425000
H	-0.546820000	-1.831338000	1.587957000
C	-3.721137000	-2.439809000	0.523100000

H	-4.756980000	-1.283534000	-0.983358000
H	-2.410826000	-3.382955000	1.965997000
H	-4.546638000	-3.139965000	0.680806000
C	1.944686000	2.446658000	-1.822497000
H	2.097720000	3.495311000	-2.137605000
H	2.872343000	2.094614000	-1.351230000
H	1.790480000	1.847464000	-2.731563000

Sum of electronic and thermal Energies= -1998.212152
Sum of electronic and thermal Enthalpies= -1998.211208
Sum of electronic and thermal Free Energies= -1998.284580
Lowest vibration frequencies (/cm^-1) : 28.4216 30.3718 35.0658

$^{2}4_{Me}$

C	3.153474000	-1.831048000	0.763245000
C	2.114135000	-0.899756000	0.886377000
C	1.324695000	-0.469960000	-0.211820000
C	1.657924000	-1.076738000	-1.450207000
C	2.701453000	-2.000203000	-1.591804000
C	3.464572000	-2.387621000	-0.483233000
H	3.728117000	-2.124148000	1.649012000
H	1.911399000	-0.489786000	1.881105000
H	1.077885000	-0.819909000	-2.341486000
H	2.916720000	-2.429073000	-2.576833000
H	4.276235000	-3.113146000	-0.586638000
Fe	-0.060278000	0.905739000	-0.019549000
C	0.749330000	2.469811000	-1.149529000
C	-0.670858000	2.426093000	-1.287986000
C	1.301893000	2.478398000	0.167494000
C	-1.504045000	2.409291000	-0.134683000
C	0.476052000	2.378809000	1.322667000
H	2.383885000	2.379669000	0.282179000
C	-0.938034000	2.359400000	1.168686000
H	-2.577939000	2.253242000	-0.255534000
H	0.929722000	2.301779000	2.313829000
H	-1.586507000	2.214972000	2.035363000
H	-1.120345000	2.392164000	-2.283924000
C	-1.397184000	-0.525282000	0.113717000
C	-2.290127000	-0.843077000	-0.941702000
C	-1.596707000	-1.273457000	1.302211000
C	-3.301788000	-1.805605000	-0.822447000
H	-2.197529000	-0.313636000	-1.895417000
C	-2.608397000	-2.231687000	1.440163000
H	-0.929674000	-1.107140000	2.153441000
C	-3.475597000	-2.508594000	0.375747000
H	-3.962811000	-2.007559000	-1.672745000
H	-2.716744000	-2.775008000	2.385449000
H	-4.263811000	-3.260078000	0.475695000
C	1.649186000	2.508407000	-2.356281000
H	1.955498000	3.542719000	-2.594292000
H	2.560372000	1.917811000	-2.193008000
H	1.144162000	2.100487000	-3.243420000

Sum of electronic and thermal Energies= -1998.252938
Sum of electronic and thermal Enthalpies= -1998.251994
Sum of electronic and thermal Free Energies= -1998.320979
Lowest vibration frequencies (/cm^-1) : 25.2900 30.9524 37.0258

$^{4}\mathbf{4}_{\mathbf{Ph}}$

C	3.788603000	-1.815638000	0.486528000
C	2.755809000	-0.875833000	0.617417000
C	1.689582000	-0.771587000	-0.305196000
C	1.727577000	-1.699261000	-1.372561000
C	2.750863000	-2.642984000	-1.525477000
C	3.793167000	-2.705728000	-0.592674000
H	4.593437000	-1.854401000	1.228366000
H	2.792504000	-0.199599000	1.479544000
H	0.920848000	-1.695406000	-2.112961000
H	2.735971000	-3.337415000	-2.371917000
H	4.595163000	-3.440835000	-0.702981000
Fe	0.140784000	0.563702000	-0.153312000
C	0.809594000	2.350087000	-0.938733000
C	-0.570080000	2.195339000	-1.385936000
C	0.957345000	2.384750000	0.489033000
C	-1.626860000	2.732834000	-0.561384000
C	-0.177039000	2.427018000	1.341876000
H	1.953602000	2.309487000	0.927302000
C	-1.446382000	2.815058000	0.802346000
H	-2.596335000	2.955283000	-1.012298000
H	-0.024908000	2.387552000	2.421109000
H	-2.265562000	3.092530000	1.468096000
H	-0.750589000	2.130723000	-2.459379000
C	-1.507569000	-0.590983000	0.070080000
C	-2.731427000	-0.504147000	-0.634875000
C	-1.435523000	-1.656038000	1.003956000
C	-3.799044000	-1.389990000	-0.426691000
H	-2.865170000	0.287331000	-1.376329000
C	-2.494456000	-2.543418000	1.234491000
H	-0.512242000	-1.808323000	1.570320000
C	-3.690469000	-2.416287000	0.517223000
H	-4.721535000	-1.279442000	-1.007148000
H	-2.384966000	-3.343317000	1.974374000
H	-4.519325000	-3.109486000	0.686490000
C	1.938966000	2.518876000	-1.869740000
C	1.919871000	1.997791000	-3.183663000
C	3.086982000	3.250971000	-1.491308000
C	2.983786000	2.195390000	-4.061890000
H	1.069490000	1.399656000	-3.508521000
C	4.156253000	3.442830000	-2.368568000
H	3.126595000	3.699528000	-0.498226000
C	4.115366000	2.919613000	-3.664773000
H	2.935510000	1.766436000	-5.065657000
H	5.025146000	4.017295000	-2.037493000
H	4.950248000	3.069164000	-4.352402000

Sum of electronic and thermal Energies= -2189.815426
Sum of electronic and thermal Enthalpies= -2189.814482
Sum of electronic and thermal Free Energies= -2189.896300
Lowest vibration frequencies (/cm^-1) : 15.6695 25.2788 28.1745

$^{2}\mathbf{4}_{\mathbf{Ph}}$

C	2.550491000	-2.539734000	1.702113000
C	1.649671000	-1.479603000	1.542008000
C	1.549842000	-0.730282000	0.343026000
C	2.413868000	-1.150830000	-0.698434000
C	3.314440000	-2.214655000	-0.554701000
C	3.396171000	-2.918526000	0.652262000
H	2.588416000	-3.080585000	2.653889000
H	0.996390000	-1.229848000	2.383450000
H	2.391263000	-0.626476000	-1.658245000
H	3.960474000	-2.494538000	-1.393667000
H	4.098556000	-3.747976000	0.770709000
Fe	0.378968000	0.830545000	0.175531000
C	0.901008000	2.439253000	-1.091692000
C	-0.452954000	2.561330000	-0.633198000
C	1.902770000	2.225839000	-0.087171000
C	-0.784747000	2.468004000	0.741493000
C	1.573196000	2.118122000	1.288304000
H	2.923397000	1.993568000	-0.394565000
C	0.217832000	2.196456000	1.712740000
H	-1.838167000	2.459345000	1.028406000
H	2.348866000	1.820326000	1.996276000
H	-0.048129000	2.050307000	2.762014000
H	-1.261625000	2.665397000	-1.357242000
C	-1.113097000	-0.388583000	-0.212077000
C	-1.293037000	-1.033453000	-1.461391000
C	-2.133106000	-0.642007000	0.739001000
C	-2.406975000	-1.830001000	-1.752832000
H	-0.529712000	-0.919624000	-2.235546000
C	-3.247880000	-1.446274000	0.466783000
H	-2.057568000	-0.192186000	1.734076000
C	-3.400504000	-2.043846000	-0.789478000
H	-2.495832000	-2.297733000	-2.739121000
H	-4.005019000	-1.606246000	1.242131000
H	-4.269447000	-2.669615000	-1.010155000
C	1.250651000	2.569595000	-2.520262000
C	2.480369000	3.142833000	-2.917086000
C	0.376525000	2.153679000	-3.550909000
C	2.820302000	3.286249000	-4.264148000
H	3.168301000	3.503657000	-2.151650000
C	0.711855000	2.307105000	-4.895518000
H	-0.563319000	1.669750000	-3.287711000
C	1.938419000	2.873473000	-5.267829000
H	3.780411000	3.735638000	-4.530319000
H	0.013347000	1.964508000	-5.662778000
H	2.201960000	2.986103000	-6.321493000

Sum of electronic and thermal Energies= -2189.858584
Sum of electronic and thermal Enthalpies= -2189.857640
Sum of electronic and thermal Free Energies= -2189.934676
Lowest vibration frequencies (/cm^-1) : 16.9621 29.0836 34.1668

^{4}5

Fe	0.061809000	0.189000000	-0.032314000
N	1.329903000	0.705691000	-1.387256000
N	-1.063058000	-0.319349000	-1.489836000
C	2.755741000	0.459339000	-1.233275000
H	3.278167000	0.757037000	-2.164017000
C	-4.573642000	2.842001000	-1.762625000
H	-5.371333000	3.215259000	-2.408761000
C	4.373656000	2.192936000	-0.302904000
H	4.849976000	2.247443000	-1.285229000
C	4.181610000	2.967579000	1.974768000
H	4.510814000	3.613425000	2.792655000
C	2.672539000	1.224025000	1.146058000
C	2.340068000	-1.730688000	-0.005280000
C	3.063974000	-1.021695000	-1.005741000
C	4.166373000	-3.090497000	-1.705670000
H	4.871301000	-3.604703000	-2.362871000
C	3.966146000	-1.709384000	-1.823308000
H	4.513051000	-1.149548000	-2.587774000
C	-1.400639000	0.035863000	1.404918000
H	-0.991266000	0.004982000	2.418806000
C	-2.291072000	-1.088262000	1.113418000
C	3.430046000	-3.801205000	-0.750555000
H	3.554021000	-4.882524000	-0.651117000
C	-2.505791000	1.850535000	-0.085278000
C	1.561549000	0.304740000	1.379270000
H	1.084771000	0.476207000	2.349904000
C	-3.963820000	3.682132000	-0.822783000
H	-4.282343000	4.723156000	-0.725969000
C	3.308071000	1.307591000	-0.114881000
C	3.121158000	2.082770000	2.173374000
H	2.632523000	2.035901000	3.150053000
C	-3.438507000	-3.107147000	1.909619000
H	-3.652590000	-3.804291000	2.723409000
C	-3.101600000	1.017565000	-1.071915000
C	4.822841000	3.021008000	0.732177000
H	5.653219000	3.710481000	0.564644000
C	-2.948328000	3.191179000	-0.002682000
H	-2.487959000	3.848891000	0.739048000
C	-1.473085000	1.359508000	0.816203000
H	-1.006763000	2.138386000	1.428586000
C	-2.594317000	-2.019609000	2.132991000
H	-2.163529000	-1.866915000	3.125515000
C	-4.010406000	-3.296781000	0.648014000
H	-4.669812000	-4.146089000	0.457238000
C	-2.857618000	-1.303312000	-0.170047000

C	-4.125053000	1.521155000	-1.880671000
H	-4.565657000	0.867129000	-2.638826000
C	0.868943000	0.297452000	-2.702728000
H	1.181218000	-0.739158000	-2.945920000
H	1.288279000	0.951624000	-3.498171000
C	2.535911000	-3.128319000	0.081107000
H	1.974094000	-3.686964000	0.833735000
C	-3.709848000	-2.392002000	-0.376960000
H	-4.132713000	-2.546078000	-1.372741000
C	-0.646654000	0.356386000	-2.697867000
H	-0.973476000	1.416614000	-2.728015000
H	-1.062515000	-0.129943000	-3.607119000
C	-2.500432000	-0.367001000	-1.306367000
H	-2.969107000	-0.769413000	-2.227588000
C	1.426364000	-1.066098000	0.916461000
H	0.924712000	-1.740766000	1.616358000

Sum of electronic and thermal Energies= -2607.542545
Sum of electronic and thermal Enthalpies= -2607.541601
Sum of electronic and thermal Free Energies= -2607.626924
Lowest vibration frequencies (/cm^-1) : 16.9621 29.0836 34.1668

^{2}5

Fe	0.000027000	-0.000079000	0.043148000
N	1.197177000	0.351838000	-1.321478000
N	-1.197163000	-0.351797000	-1.321499000
C	2.640032000	0.279198000	-1.158373000
H	3.135424000	0.528959000	-2.115687000
C	-4.439076000	3.123515000	-1.086000000
H	-5.217034000	3.654398000	-1.639625000
C	4.127624000	2.195802000	-0.405040000
H	4.613016000	2.163424000	-1.384153000
C	3.867760000	3.211376000	1.766109000
H	4.149807000	3.963271000	2.507569000
C	2.462143000	1.299898000	1.135812000
C	2.396863000	-1.740974000	0.313168000
C	3.088865000	-1.119139000	-0.755021000
C	4.439456000	-3.123222000	-1.086410000
H	5.217518000	-3.653931000	-1.640053000
C	4.102217000	-1.807888000	-1.428445000
H	4.623633000	-1.311861000	-2.251768000
C	-1.403776000	-0.353561000	1.476173000
H	-0.965362000	-0.550816000	2.462781000
C	-2.462164000	-1.300138000	1.135671000
C	3.751162000	-3.753501000	-0.045785000
H	3.992258000	-4.782765000	0.231120000
C	-2.396712000	1.740841000	0.313492000
C	1.403853000	0.353173000	1.476204000
H	0.965456000	0.550243000	2.462857000
C	-3.750792000	3.753558000	-0.045227000
H	-3.991792000	4.782807000	0.231817000
C	3.108502000	1.280435000	-0.125560000

C	2.860364000	2.292128000	2.060073000
H	2.369661000	2.324308000	3.036222000
C	-3.868142000	-3.211400000	1.765814000
H	-4.150319000	-3.963313000	2.507207000
C	-3.088728000	1.119235000	-0.754821000
C	4.516906000	3.163835000	0.527756000
H	5.304441000	3.879949000	0.283214000
C	-2.748267000	3.065464000	0.643118000
H	-2.221758000	3.558167000	1.464347000
C	-1.349561000	1.043433000	1.078437000
H	-0.875374000	1.698719000	1.817663000
C	-2.860513000	-2.292420000	2.059821000
H	-2.369765000	-2.324817000	3.035941000
C	-4.517373000	-3.163549000	0.527518000
H	-5.305110000	-3.879432000	0.282955000
C	-3.108575000	-1.280399000	-0.125666000
C	-4.101965000	1.808192000	-1.428205000
H	-4.623377000	1.312347000	-2.251639000
C	0.751272000	-0.097781000	-2.624028000
H	0.986269000	-1.170688000	-2.796296000
H	1.232790000	0.471872000	-3.446181000
C	2.748519000	-3.065618000	0.642599000
H	2.222020000	-3.558498000	1.463728000
C	-4.127917000	-2.195507000	-0.405195000
H	-4.613378000	-2.162887000	-1.384265000
C	-0.751281000	0.098008000	-2.623994000
H	-0.986277000	1.170941000	-2.796099000
H	-1.232822000	-0.471522000	-3.446219000
C	-2.640012000	-0.279085000	-1.158361000
H	-3.135434000	-0.528682000	-2.115703000
C	1.349673000	-1.043749000	1.078225000
H	0.875519000	-1.699174000	1.817349000

Sum of electronic and thermal Energies= -2607.570492
Sum of electronic and thermal Enthalpies= -2607.569548
Sum of electronic and thermal Free Energies= -2607.651540
Lowest vibration frequencies (/cm^-1) : 31.3694 41.3394 48.6840

^{4}6 (computed at the OPBE-d3bj level)

Fe	0.996951000	0.132110000	0.007201000
C	1.413617000	1.411478000	3.983768000
C	1.792785000	0.099372000	4.132784000
C	4.718134000	-1.657637000	-0.625030000
C	5.132202000	-0.440071000	-0.147070000
C	-2.822921000	1.824802000	-0.048821000
C	-3.031282000	0.824361000	0.866677000
C	-0.110148000	-0.949830000	-3.899645000
C	0.882915000	-0.044678000	-4.186532000
C	-0.832111000	0.693142000	0.195516000
C	2.829904000	-0.418148000	-0.178740000
C	1.280378000	0.419359000	1.920971000
C	0.708196000	-0.172180000	-1.904097000

C	0.574941000	2.788828000	2.016985000
H	0.571181000	2.508750000	0.950737000
C	2.085599000	-1.840892000	2.514679000
H	1.764786000	-1.893756000	1.461709000
C	2.487988000	1.316260000	-2.756673000
H	2.448546000	1.473561000	-1.665873000
C	-1.175392000	-1.763683000	-1.737575000
H	-0.823434000	-1.592955000	-0.706851000
C	3.914144000	1.619475000	0.707325000
H	2.836255000	1.843140000	0.631393000
C	2.445013000	-2.668242000	-1.134022000
H	1.453139000	-2.279194000	-0.848010000
C	-1.538030000	-0.942098000	1.913998000
H	-0.516567000	-1.228491000	1.611072000
C	-0.833771000	2.528050000	-1.462382000
H	0.213087000	2.192549000	-1.370229000
N	-1.819075000	0.155739000	1.000454000
N	-1.492110000	1.728060000	-0.440171000
N	-0.203414000	-1.003734000	-2.513662000
N	1.366327000	0.408057000	-2.964527000
N	1.711106000	-0.478265000	2.871373000
N	1.103274000	1.580863000	2.639826000
N	3.327964000	-1.623827000	-0.635042000
N	3.978974000	0.291305000	0.116110000
C	2.154507000	-0.610984000	5.381968000
H	3.038714000	-1.244084000	5.264939000
H	2.375918000	0.115604000	6.169598000
H	1.332688000	-1.247153000	5.737681000
C	1.393631000	2.477948000	5.012155000
H	2.255839000	3.151487000	4.913461000
H	0.487192000	3.088333000	4.967737000
H	1.436576000	2.029781000	6.009470000
C	-4.297142000	0.450400000	1.540298000
H	-5.025355000	1.260502000	1.436088000
H	-4.739572000	-0.452115000	1.097195000
H	-4.168429000	0.265124000	2.610862000
C	-3.779038000	2.861545000	-0.503692000
H	-3.556602000	3.841091000	-0.059237000
H	-3.783851000	2.983527000	-1.591134000
H	-4.794239000	2.585441000	-0.203115000
C	-0.894487000	-1.778770000	-4.844490000
H	-0.775676000	-1.393305000	-5.861576000
H	-0.552531000	-2.822373000	-4.842976000
H	-1.964987000	-1.778848000	-4.618374000
C	1.333723000	0.430222000	-5.515572000
H	0.966433000	1.443154000	-5.727802000
H	2.423681000	0.443684000	-5.610214000
H	0.946665000	-0.232102000	-6.295718000
C	6.519287000	0.055933000	0.012033000
H	6.690948000	0.521576000	0.987279000
H	7.222047000	-0.777928000	-0.078303000

H	6.778561000	0.792550000	-0.760132000
C	5.550696000	-2.824973000	-1.000227000
H	5.238909000	-3.277550000	-1.946307000
H	6.593521000	-2.514275000	-1.115747000
H	5.520929000	-3.607845000	-0.230422000
C	4.675352000	2.676468000	-0.072182000
H	4.365112000	3.665372000	0.286908000
H	5.757509000	2.602678000	0.069479000
H	4.453534000	2.618879000	-1.139881000
C	4.307158000	1.591746000	2.172773000
H	4.148231000	2.576723000	2.623279000
H	3.708133000	0.865774000	2.722236000
H	5.365078000	1.340540000	2.300972000
C	2.643374000	-4.013298000	-0.457918000
H	1.786405000	-4.653505000	-0.700448000
H	3.544109000	-4.527767000	-0.804969000
H	2.692047000	-3.908999000	0.628169000
C	2.511909000	-2.769832000	-2.646736000
H	1.801734000	-3.522731000	-3.004009000
H	2.262335000	-1.816043000	-3.110864000
H	3.507926000	-3.071537000	-2.986204000
C	3.803717000	0.645774000	-3.103664000
H	4.638136000	1.306637000	-2.848203000
H	3.921281000	-0.282384000	-2.544416000
H	3.875309000	0.423913000	-4.173455000
C	2.318759000	2.658968000	-3.442479000
H	3.077555000	3.347249000	-3.051343000
H	2.460760000	2.596482000	-4.524957000
H	1.335241000	3.087258000	-3.237979000
C	-1.142204000	-3.255324000	-2.015623000
H	-1.711727000	-3.767815000	-1.231010000
H	-1.601500000	-3.512628000	-2.974424000
H	-0.119462000	-3.638094000	-1.998834000
C	-2.565969000	-1.174198000	-1.880895000
H	-3.274778000	-1.733698000	-1.261791000
H	-2.578048000	-0.133111000	-1.558282000
H	-2.922258000	-1.226022000	-2.914683000
C	-0.854351000	3.051850000	2.452044000
H	-0.915715000	3.312521000	3.513724000
H	-1.266403000	3.891510000	1.883301000
H	-1.480382000	2.178716000	2.268168000
C	1.469470000	4.002159000	2.189351000
H	1.115425000	4.793151000	1.517442000
H	1.443123000	4.401669000	3.207121000
H	2.503814000	3.771479000	1.925973000
C	1.333258000	-2.900162000	3.298780000
H	1.501191000	-3.872678000	2.820686000
H	1.679111000	-2.978992000	4.333192000
H	0.259247000	-2.702449000	3.299111000
C	3.589933000	-2.028370000	2.575710000
H	3.853587000	-3.034703000	2.234903000

H	4.095523000	-1.308160000	1.932444000
H	3.971098000	-1.917247000	3.595892000
C	-2.448480000	-2.141903000	1.722777000
H	-2.006160000	-3.002450000	2.239335000
H	-3.444452000	-1.982834000	2.146059000
H	-2.550720000	-2.394959000	0.665725000
C	-1.506076000	-0.468760000	3.355305000
H	-1.244915000	-1.301289000	4.016831000
H	-0.767666000	0.321336000	3.490009000
H	-2.481927000	-0.089870000	3.675287000
C	-0.880141000	4.021638000	-1.195213000
H	-0.159077000	4.516814000	-1.856969000
H	-1.863419000	4.453830000	-1.402096000
H	-0.603478000	4.247855000	-0.163192000
C	-1.340669000	2.172862000	-2.847500000
H	-0.766622000	2.711651000	-3.608141000
H	-1.237307000	1.104290000	-3.033205000
H	-2.392833000	2.447611000	-2.973302000

Sum of electronic and thermal Energies= -3425.327060
Sum of electronic and thermal Enthalpies= -3425.326116
Sum of electronic and thermal Free Energies= -3425.482701
Lowest vibration frequencies (/cm^-1) : 28.6543 44.4928 50.2903

^{2}**6** (computed at the OPBE-d3bj level)

Fe	0.997847000	0.129759000	0.007274000
C	1.422192000	1.412890000	3.953892000
C	1.761225000	0.092574000	4.108616000
C	4.712073000	-1.663661000	-0.613464000
C	5.126026000	-0.434679000	-0.165811000
C	-2.812224000	1.824990000	-0.037622000
C	-3.029266000	0.804223000	0.852900000
C	-0.087296000	-0.957896000	-3.871171000
C	0.879684000	-0.028391000	-4.160060000
C	-0.824020000	0.681763000	0.193546000
C	2.821350000	-0.420069000	-0.177598000
C	1.275427000	0.419238000	1.879359000
C	0.718298000	-0.159985000	-1.864667000
C	0.600304000	2.787712000	1.976286000
H	0.571962000	2.499460000	0.916733000
C	2.044603000	-1.843171000	2.481232000
H	1.751898000	-1.886079000	1.423528000
C	2.471716000	1.342129000	-2.721883000
H	2.451083000	1.476028000	-1.631731000
C	-1.140423000	-1.769180000	-1.700258000
H	-0.804054000	-1.577338000	-0.672334000
C	3.891995000	1.617334000	0.699330000
H	2.813993000	1.824368000	0.654188000
C	2.425007000	-2.657563000	-1.126353000
H	1.438185000	-2.245383000	-0.875269000
C	-1.515610000	-0.948726000	1.907442000
H	-0.483425000	-1.205886000	1.633467000

C	-0.812042000	2.515127000	-1.452411000
H	0.222825000	2.151883000	-1.385425000
N	-1.816280000	0.132408000	0.979288000
N	-1.477790000	1.728994000	-0.423112000
N	-0.169262000	-1.017058000	-2.482390000
N	1.351999000	0.435624000	-2.935256000
N	1.668840000	-0.484298000	2.844900000
N	1.130202000	1.584985000	2.603552000
N	3.320301000	-1.629898000	-0.613878000
N	3.969501000	0.296058000	0.092849000
C	2.086510000	-0.630493000	5.360357000
H	2.977915000	-1.258918000	5.268200000
H	2.277032000	0.087337000	6.163842000
H	1.256767000	-1.274483000	5.682234000
C	1.436933000	2.488039000	4.973251000
H	2.303289000	3.151812000	4.846999000
H	0.536286000	3.109264000	4.949639000
H	1.502305000	2.048706000	5.973247000
C	-4.301560000	0.403399000	1.497511000
H	-5.043620000	1.198805000	1.378924000
H	-4.715514000	-0.505175000	1.038952000
H	-4.195694000	0.214989000	2.570550000
C	-3.754040000	2.885433000	-0.465635000
H	-3.496469000	3.855865000	-0.020360000
H	-3.783890000	3.015616000	-1.552298000
H	-4.767631000	2.632457000	-0.140423000
C	-0.852383000	-1.810715000	-4.810272000
H	-0.722543000	-1.444987000	-5.833323000
H	-0.501753000	-2.851286000	-4.784553000
H	-1.926824000	-1.816405000	-4.600573000
C	1.307568000	0.469797000	-5.488050000
H	0.939930000	1.487928000	-5.674193000
H	2.395785000	0.481589000	-5.607538000
H	0.901461000	-0.175030000	-6.273199000
C	6.509691000	0.080356000	-0.044577000
H	6.701802000	0.558466000	0.921187000
H	7.221533000	-0.744419000	-0.146527000
H	6.737830000	0.812604000	-0.830738000
C	5.540524000	-2.842475000	-0.958702000
H	5.255151000	-3.296968000	-1.912819000
H	6.590407000	-2.545353000	-1.040609000
H	5.476459000	-3.620447000	-0.186054000
C	4.629183000	2.694706000	-0.075453000
H	4.319887000	3.676598000	0.302235000
H	5.713361000	2.623882000	0.051003000
H	4.395806000	2.650521000	-1.140877000
C	4.305548000	1.574573000	2.159257000
H	4.146307000	2.552803000	2.623998000
H	3.714826000	0.839014000	2.705449000
H	5.366131000	1.326543000	2.267934000
C	2.580687000	-4.004533000	-0.443828000

H	1.728931000	-4.638944000	-0.716703000
H	3.489212000	-4.524258000	-0.761195000
H	2.594949000	-3.902503000	0.643096000
C	2.523015000	-2.763312000	-2.637594000
H	1.788488000	-3.483243000	-3.012468000
H	2.323985000	-1.798422000	-3.104163000
H	3.513026000	-3.108916000	-2.951021000
C	3.786501000	0.679414000	-3.091418000
H	4.624215000	1.336841000	-2.837894000
H	3.909105000	-0.255724000	-2.544632000
H	3.842813000	0.471325000	-4.164474000
C	2.298931000	2.695863000	-3.385552000
H	3.059419000	3.382183000	-2.994583000
H	2.433434000	2.641945000	-4.469386000
H	1.315569000	3.119669000	-3.173325000
C	-1.107543000	-3.265356000	-1.955265000
H	-1.683213000	-3.770851000	-1.170785000
H	-1.561909000	-3.529294000	-2.914588000
H	-0.086600000	-3.651105000	-1.932281000
C	-2.534541000	-1.188994000	-1.856752000
H	-3.233606000	-1.706938000	-1.192384000
H	-2.540462000	-0.130160000	-1.597662000
H	-2.903224000	-1.304298000	-2.880712000
C	-0.823780000	3.059420000	2.427077000
H	-0.867707000	3.315826000	3.490225000
H	-1.239448000	3.903003000	1.866773000
H	-1.455403000	2.188922000	2.248472000
C	1.496415000	4.003106000	2.129383000
H	1.143169000	4.791353000	1.454066000
H	1.471264000	4.407805000	3.145099000
H	2.530802000	3.769770000	1.869994000
C	1.283297000	-2.912753000	3.243168000
H	1.455046000	-3.882194000	2.760502000
H	1.621383000	-2.998579000	4.279551000
H	0.209695000	-2.715268000	3.239376000
C	3.548372000	-2.034594000	2.564532000
H	3.819138000	-3.037967000	2.220527000
H	4.062752000	-1.307969000	1.935413000
H	3.909240000	-1.929912000	3.592376000
C	-2.390437000	-2.175510000	1.723659000
H	-1.955154000	-3.008745000	2.288108000
H	-3.404454000	-2.019383000	2.102516000
H	-2.448813000	-2.468572000	0.673778000
C	-1.511525000	-0.451925000	3.341862000
H	-1.211626000	-1.259335000	4.017522000
H	-0.807728000	0.372126000	3.461183000
H	-2.504905000	-0.113081000	3.651711000
C	-0.823148000	4.009663000	-1.186958000
H	-0.110667000	4.494720000	-1.864774000
H	-1.804690000	4.454614000	-1.373506000
H	-0.523518000	4.233984000	-0.161462000

C	-1.343743000	2.169564000	-2.831254000
H	-0.777562000	2.707298000	-3.598429000
H	-1.246360000	1.100930000	-3.021915000
H	-2.395777000	2.451830000	-2.937221000

Sum of electronic and thermal Energies= -3425.383814
Sum of electronic and thermal Enthalpies= -3425.382870
Sum of electronic and thermal Free Energies= -3425.536720
Lowest vibration frequencies (/cm^-1) : 41.2590 53.0992 57.2653

^{4}7

Fe	-1.265074000	-0.431000000	-0.389362000
N	-3.122522000	-0.610607000	-0.019341000
C	-3.915027000	0.301596000	0.655325000
C	-3.892583000	-1.739218000	-0.240701000
C	-5.167087000	-0.250435000	0.879329000
C	-5.152805000	-1.554201000	0.307140000
H	-6.006304000	0.232644000	1.374700000
H	-5.978725000	-2.261452000	0.280232000
P	-1.468497000	-2.622694000	-1.034312000
P	-1.517981000	1.540724000	0.762997000
C	-3.370571000	1.669746000	0.886143000
H	-3.695919000	2.106831000	1.840552000
H	-3.709845000	2.357921000	0.094802000
C	-3.317931000	-2.823737000	-1.085940000
H	-3.633634000	-2.705127000	-2.135648000
H	-3.639471000	-3.827389000	-0.775467000
C	0.164755000	0.588517000	-2.710828000
C	-2.153488000	0.729435000	-3.115750000
C	0.406327000	1.145575000	-4.001456000
C	-1.975774000	1.272586000	-4.382756000
H	-3.154532000	0.546504000	-2.720327000
C	-0.645589000	1.483335000	-4.828045000
H	1.429393000	1.306474000	-4.339039000
H	-2.837118000	1.523183000	-5.000267000
H	-0.451195000	1.908212000	-5.814300000
C	1.165971000	0.198751000	-1.773603000
C	1.591482000	-0.721708000	0.365281000
C	2.572841000	0.305633000	-1.971975000
C	2.967023000	-0.632577000	0.215107000
H	1.165538000	-1.129146000	1.283365000
C	3.466542000	-0.097214000	-1.002969000
H	2.945561000	0.716324000	-2.909211000
H	3.626496000	-0.967563000	1.014035000
H	4.540250000	-0.005451000	-1.172056000
N	0.695528000	-0.331525000	-0.565084000
N	-1.146451000	0.391804000	-2.291047000
C	-0.926947000	3.133040000	-0.062152000
C	-1.750274000	4.417651000	0.141570000
C	0.567514000	3.408897000	0.184417000
H	-1.027603000	2.855770000	-1.124451000
C	-1.234623000	5.541478000	-0.766809000

H	-1.699107000	4.751163000	1.188302000
H	-2.812507000	4.245077000	-0.078904000
C	1.077419000	4.538764000	-0.717071000
H	0.726735000	3.698280000	1.234800000
H	1.162910000	2.504956000	0.009579000
C	0.253635000	5.815367000	-0.551513000
H	-1.823653000	6.455586000	-0.589134000
H	-1.405819000	5.260432000	-1.819761000
H	2.138254000	4.734949000	-0.493979000
H	1.036360000	4.207236000	-1.767569000
H	0.603164000	6.590520000	-1.251719000
H	0.406812000	6.221436000	0.463318000
C	-0.900896000	1.562288000	2.544767000
C	-1.220535000	2.799967000	3.399116000
C	-1.359319000	0.291508000	3.279076000
H	0.195215000	1.501573000	2.426924000
C	-0.603100000	2.690030000	4.799933000
H	-2.311993000	2.911033000	3.498577000
H	-0.853373000	3.715244000	2.919850000
C	-0.739533000	0.180980000	4.675054000
H	-2.457033000	0.288195000	3.364664000
H	-1.101911000	-0.595264000	2.687097000
C	-1.036923000	1.416372000	5.523680000
H	-0.876031000	3.579548000	5.390045000
H	0.496699000	2.702646000	4.711370000
H	-1.114442000	-0.727051000	5.173366000
H	0.353067000	0.057146000	4.580586000
H	-0.535300000	1.342718000	6.501381000
H	-2.119565000	1.463842000	5.731112000
C	-0.832011000	-3.102460000	-2.746606000
C	0.672181000	-3.431230000	-2.746644000
C	-1.613880000	-4.152961000	-3.555667000
H	-0.946014000	-2.143388000	-3.278100000
C	1.214414000	-3.542340000	-4.176018000
H	0.846941000	-4.386707000	-2.228040000
H	1.235878000	-2.664849000	-2.200935000
C	-1.064264000	-4.253175000	-4.984545000
H	-1.548497000	-5.140991000	-3.077648000
H	-2.681654000	-3.899511000	-3.604406000
C	0.432622000	-4.561985000	-5.003446000
H	2.282128000	-3.811272000	-4.142962000
H	1.156167000	-2.553650000	-4.659961000
H	-1.622930000	-5.024344000	-5.538946000
H	-1.246526000	-3.299538000	-5.508282000
H	0.803920000	-4.580007000	-6.040348000
H	0.602670000	-5.573445000	-4.595267000
C	-0.860323000	-3.930970000	0.182557000
C	-1.353084000	-3.611134000	1.603573000
C	-1.157041000	-5.401494000	-0.152400000
H	0.235125000	-3.792746000	0.171437000
C	-0.746316000	-4.557316000	2.644179000

H	-2.450978000	-3.682331000	1.640807000
H	-1.112044000	-2.571558000	1.857412000
C	-0.555724000	-6.351993000	0.891552000
H	-2.246207000	-5.560920000	-0.193179000
H	-0.762668000	-5.665111000	-1.140643000
C	-1.024046000	-6.021748000	2.307745000
H	-1.143527000	-4.310548000	3.641512000
H	0.344326000	-4.395216000	2.693604000
H	-0.815953000	-7.390752000	0.632287000
H	0.544979000	-6.288400000	0.846567000
H	-0.532851000	-6.684187000	3.037737000
H	-2.107087000	-6.215769000	2.389450000

Sum of electronic and thermal Energies= -3668.461023
Sum of electronic and thermal Enthalpies= -3668.460078
Sum of electronic and thermal Free Energies= -3668.587693
Lowest vibration frequencies (/cm^-1): 7.2292 19.6049 35.5734

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Fe	-1.158569000	-0.354047000	-0.556911000
N	-3.056944000	-0.546528000	-0.158127000
C	-3.840117000	0.351916000	0.528166000
C	-3.822945000	-1.670301000	-0.365383000
C	-5.099430000	-0.198739000	0.767508000
C	-5.088466000	-1.494369000	0.194963000
H	-5.928373000	0.283529000	1.281246000
H	-5.906390000	-2.211644000	0.181187000
P	-1.385539000	-2.614148000	-0.993638000
P	-1.427066000	1.520143000	0.765369000
C	-3.278653000	1.707939000	0.786288000
H	-3.649656000	2.156727000	1.718194000
H	-3.541277000	2.407660000	-0.025602000
C	-3.231707000	-2.770797000	-1.177198000
H	-3.459911000	-2.644348000	-2.249399000
H	-3.605086000	-3.764616000	-0.892468000
C	-0.138703000	0.692669000	-2.971844000
C	-2.477425000	0.665471000	-3.013302000
C	-0.108015000	1.246489000	-4.263171000
C	-2.505476000	1.210604000	-4.285589000
H	-3.391266000	0.418817000	-2.475747000
C	-1.293810000	1.512118000	-4.937009000
H	0.847521000	1.469009000	-4.737503000
H	-3.466657000	1.398655000	-4.765421000
H	-1.282393000	1.940920000	-5.939154000
C	1.018828000	0.367833000	-2.160821000
C	1.701263000	-0.510130000	-0.098807000
C	2.361495000	0.553619000	-2.529114000
C	3.039789000	-0.347682000	-0.414482000
H	1.393767000	-0.932479000	0.856773000
C	3.389406000	0.200216000	-1.662285000
H	2.597155000	0.978941000	-3.503857000
H	3.799672000	-0.646861000	0.307866000

H	4.432336000	0.343031000	-1.944716000
N	0.674844000	-0.167287000	-0.929803000
N	-1.328287000	0.394751000	-2.332661000
C	-0.749992000	3.128333000	0.020518000
C	-1.564114000	4.423181000	0.196549000
C	0.725777000	3.377824000	0.377013000
H	-0.780719000	2.885861000	-1.054775000
C	-0.968376000	5.563080000	-0.639642000
H	-1.584961000	4.728424000	1.252593000
H	-2.609612000	4.273380000	-0.104029000
C	1.319097000	4.523045000	-0.451762000
H	0.814043000	3.635302000	1.444240000
H	1.321047000	2.469198000	0.222394000
C	0.503937000	5.808074000	-0.311051000
H	-1.554850000	6.482001000	-0.478686000
H	-1.067927000	5.315428000	-1.710317000
H	2.363792000	4.695500000	-0.146731000
H	1.350913000	4.223278000	-1.512518000
H	0.915013000	6.596336000	-0.961603000
H	0.589001000	6.183382000	0.723380000
C	-0.892750000	1.525835000	2.580455000
C	-1.326293000	2.714738000	3.453486000
C	-1.290850000	0.203933000	3.254066000
H	0.209324000	1.542065000	2.513996000
C	-0.770632000	2.601382000	4.879401000
H	-2.425419000	2.756532000	3.505615000
H	-0.995354000	3.665222000	3.017759000
C	-0.739387000	0.093826000	4.678210000
H	-2.387862000	0.112515000	3.273449000
H	-0.927905000	-0.634495000	2.647179000
C	-1.159891000	1.281343000	5.543168000
H	-1.126749000	3.453816000	5.480168000
H	0.329616000	2.683240000	4.847854000
H	-1.077569000	-0.851080000	5.132560000
H	0.362875000	0.044317000	4.640055000
H	-0.707537000	1.208572000	6.544944000
H	-2.252862000	1.255467000	5.691276000
C	-0.659096000	-3.170249000	-2.652813000
C	0.831194000	-3.543343000	-2.564112000
C	-1.423326000	-4.221099000	-3.478877000
H	-0.714977000	-2.226948000	-3.221496000
C	1.449253000	-3.711354000	-3.957434000
H	0.948667000	-4.487367000	-2.009655000
H	1.388713000	-2.779998000	-2.007515000
C	-0.802802000	-4.376074000	-4.873212000
H	-1.411824000	-5.196908000	-2.973302000
H	-2.479472000	-3.941006000	-3.589222000
C	0.683095000	-4.728104000	-4.802981000
H	2.504926000	-4.011601000	-3.859235000
H	1.450186000	-2.735381000	-4.470702000
H	-1.353003000	-5.146215000	-5.437531000

H	-0.928668000	-3.432766000	-5.431581000
H	1.111289000	-4.783276000	-5.816529000
H	0.799844000	-5.733048000	-4.361864000
C	-0.900130000	-3.927999000	0.278902000
C	-1.497500000	-3.578316000	1.651346000
C	-1.198443000	-5.397357000	-0.058835000
H	0.196309000	-3.814905000	0.355292000
C	-0.996935000	-4.519540000	2.750689000
H	-2.595886000	-3.628869000	1.599936000
H	-1.259397000	-2.539048000	1.904493000
C	-0.707922000	-6.345076000	1.044616000
H	-2.283228000	-5.534970000	-0.190406000
H	-0.727365000	-5.686990000	-1.005439000
C	-1.281246000	-5.982495000	2.413376000
H	-1.467675000	-4.248904000	3.709289000
H	0.089778000	-4.380645000	2.887255000
H	-0.970452000	-7.382006000	0.779430000
H	0.394276000	-6.307344000	1.089519000
H	-0.868396000	-6.646208000	3.189581000
H	-2.371921000	-6.148452000	2.407672000

Sum of electronic and thermal Energies= -3668.466607
Sum of electronic and thermal Enthalpies= -3668.465662
Sum of electronic and thermal Free Energies= -3668.592733
Lowest vibration frequencies (/cm^-1): 7.5712 18.2658 21.7444

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Fe	-0.864018000	-0.046212000	0.024178000
C	-2.458300000	-0.046464000	1.459490000
C	-2.450944000	1.196489000	0.766995000
C	-2.482033000	-1.267437000	0.728290000
C	-2.462429000	1.218360000	-0.653531000
H	-2.379936000	2.129275000	1.321131000
C	-2.491071000	-1.245709000	-0.692215000
H	-2.433633000	-2.218408000	1.252758000
C	-2.478495000	-0.002434000	-1.384780000
H	-2.401080000	2.168447000	-1.178365000
H	-2.447630000	-2.180020000	-1.246985000
H	-2.466590000	0.012905000	-2.472864000
H	-2.434670000	-0.063114000	2.547398000
C	1.196111000	-0.060933000	0.000015000
C	1.907483000	1.179084000	-0.049055000
C	1.930169000	-1.295832000	0.024206000
C	3.326714000	1.186321000	-0.117508000
C	3.353221000	-1.292829000	0.027243000
C	3.981936000	-0.043788000	-0.075132000
H	5.072652000	-0.039338000	-0.120429000
C	1.131595000	-2.581782000	-0.008439000
C	0.721577000	-3.236475000	1.190300000
C	0.776104000	-3.164603000	-1.261223000
C	-0.089480000	-4.379025000	1.107882000
C	-0.041228000	-4.305399000	-1.276073000

C	-0.500956000	-4.928831000	-0.111448000
H	-0.394242000	-4.866851000	2.034560000
H	-0.318139000	-4.742291000	-2.237419000
C	1.138190000	2.485645000	-0.013062000
C	0.823463000	3.098786000	1.237503000
C	0.732442000	3.149183000	-1.207863000
C	0.040868000	4.263050000	1.261441000
C	-0.047640000	4.313465000	-1.117854000
C	-0.427258000	4.885810000	0.098978000
H	-0.194766000	4.709431000	2.228349000
H	-0.358365000	4.807659000	-2.040630000
C	4.193171000	2.439717000	-0.230800000
H	3.520976000	3.308595000	-0.256979000
C	5.028202000	2.448188000	-1.523202000
H	5.804511000	1.670245000	-1.503143000
H	4.412924000	2.275022000	-2.413243000
H	5.539424000	3.415053000	-1.643812000
C	5.130964000	2.616159000	0.975901000
H	5.906642000	1.837665000	0.997709000
H	5.644938000	3.587714000	0.922795000
H	4.590969000	2.569361000	1.927610000
C	4.369863000	-2.446423000	0.152910000
H	5.164912000	-2.178143000	-0.565363000
C	5.041454000	-2.422159000	1.540450000
H	5.869240000	-3.146480000	1.575173000
H	5.451849000	-1.432031000	1.777723000
H	4.334462000	-2.685237000	2.335339000
C	3.970321000	-3.875129000	-0.213057000
H	3.226382000	-4.305687000	0.463330000
H	3.571171000	-3.934029000	-1.228305000
H	4.866014000	-4.513414000	-0.173475000
C	1.289265000	-2.629434000	-2.601109000
H	2.117119000	-1.943372000	-2.376482000
C	1.183275000	-2.789935000	2.579431000
H	1.924134000	-1.992929000	2.432538000
C	1.838537000	-3.725508000	-3.531331000
H	2.373012000	-3.261854000	-4.373521000
H	2.536171000	-4.403006000	-3.024346000
H	1.036423000	-4.340706000	-3.962929000
C	0.230954000	-1.817785000	-3.357484000
H	-0.108509000	-0.968692000	-2.757780000
H	0.645014000	-1.428141000	-4.299554000
H	-0.643396000	-2.436541000	-3.607928000
C	1.863218000	-3.925477000	3.364520000
H	2.330911000	-3.524709000	4.276029000
H	1.140871000	-4.689559000	3.684045000
H	2.640844000	-4.430989000	2.780196000
C	0.054863000	-2.196974000	3.432850000
H	-0.386125000	-1.322561000	2.946974000
H	-0.744266000	-2.930461000	3.614910000
H	0.442702000	-1.880958000	4.412784000

C	-1.358917000	-6.184118000	-0.189621000
H	-1.580255000	-6.349683000	-1.257226000
C	-0.597780000	-7.423762000	0.306228000
H	-1.204652000	-8.331752000	0.173204000
H	0.341599000	-7.557830000	-0.247609000
H	-0.347002000	-7.343256000	1.373505000
C	-2.708139000	-6.032951000	0.527326000
H	-2.581968000	-5.889983000	1.609890000
H	-3.272665000	-5.173973000	0.138465000
H	-3.323919000	-6.933094000	0.384203000
C	1.172748000	2.711891000	-2.604897000
H	1.804426000	1.821396000	-2.486934000
C	1.364498000	2.586984000	2.573104000
H	2.037215000	1.747925000	2.352099000
C	2.184797000	3.666134000	3.302149000
H	2.719992000	3.223950000	4.155653000
H	2.923578000	4.137179000	2.642813000
H	1.543452000	4.464764000	3.701913000
C	0.271576000	2.053968000	3.508167000
H	-0.273883000	1.227222000	3.043823000
H	0.715760000	1.684101000	4.444286000
H	-0.452735000	2.837619000	3.774013000
C	2.015720000	3.805901000	-3.286074000
H	2.459585000	3.422168000	-4.216730000
H	1.402039000	4.677876000	-3.553387000
H	2.828401000	4.161801000	-2.642960000
C	0.009098000	2.328566000	-3.529572000
H	-0.582741000	1.509551000	-3.111539000
H	-0.664269000	3.178767000	-3.711118000
H	0.393474000	2.001786000	-4.507072000
C	-1.260413000	6.159063000	0.134258000
H	-1.519823000	6.396125000	-0.911071000
C	-0.458017000	7.351633000	0.677440000
H	0.464106000	7.503011000	0.099564000
H	-1.050994000	8.276623000	0.622095000
H	-0.172137000	7.201071000	1.728010000
C	-2.583796000	5.982078000	0.892831000
H	-3.176095000	5.157046000	0.472868000
H	-2.417944000	5.768299000	1.958259000
H	-3.190321000	6.897667000	0.831257000

Sum of electronic and thermal Energies= -3131.578513
Sum of electronic and thermal Enthalpies= -3131.577569
Sum of electronic and thermal Free Energies= -3131.725001
Lowest vibration frequencies (/cm^-1) : 21.8414 23.9772 25.9094

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Fe	-0.487969000	-0.660782000	-0.007108000
C	-1.918055000	0.514415000	0.841485000
C	-1.940822000	0.661560000	-0.574936000
C	-2.004208000	-0.771804000	1.429431000
C	-2.068917000	-0.479045000	-1.404251000

H	-1.836397000	1.650278000	-1.010453000
C	-2.091747000	-1.911088000	0.592294000
H	-1.952252000	-0.890264000	2.509948000
C	-2.130078000	-1.764817000	-0.814644000
H	-2.096551000	-0.367206000	-2.487032000
H	-2.053283000	-2.907045000	1.027166000
H	-2.131095000	-2.653190000	-1.444368000
H	-1.787078000	1.397272000	1.456758000
C	1.102968000	0.520538000	0.083185000
C	1.480334000	1.901813000	0.111309000
C	2.103244000	-0.484346000	0.139609000
C	2.864970000	2.215969000	0.214573000
C	3.489885000	-0.190041000	0.178081000
C	3.799391000	1.175612000	0.239602000
H	4.855443000	1.444309000	0.302993000
C	1.430998000	-1.839710000	0.216463000
C	1.264293000	-2.492390000	1.499757000
C	1.051727000	-2.556410000	-0.974054000
C	0.706872000	-3.771609000	1.545442000
C	0.480965000	-3.843595000	-0.836008000
C	0.304337000	-4.472856000	0.392301000
H	0.609780000	-4.259677000	2.514013000
H	0.216308000	-4.392835000	-1.741327000
C	0.458795000	3.013815000	-0.000587000
C	-0.140649000	3.613040000	1.148609000
C	0.066544000	3.489257000	-1.286106000
C	-1.199027000	4.519249000	0.978969000
C	-0.995339000	4.402032000	-1.390176000
C	-1.674060000	4.907402000	-0.278183000
H	-1.657575000	4.951049000	1.869114000
H	-1.304815000	4.738036000	-2.381884000
C	3.420047000	3.639107000	0.289588000
H	2.564885000	4.328718000	0.269539000
C	4.317044000	3.986049000	-0.910753000
H	5.249707000	3.404369000	-0.898569000
H	3.818971000	3.790574000	-1.866273000
H	4.596003000	5.050202000	-0.884214000
C	4.199705000	3.889108000	1.591977000
H	5.134582000	3.311616000	1.617617000
H	4.471654000	4.951754000	1.678187000
H	3.619063000	3.614352000	2.479773000
C	4.728869000	-1.097495000	0.105565000
H	5.453701000	-0.631033000	0.795977000
C	4.619188000	-2.553176000	0.558454000
H	5.596696000	-3.043639000	0.439116000
H	4.350934000	-2.624020000	1.616407000
H	3.887449000	-3.131321000	-0.013154000
C	5.373360000	-1.004118000	-1.291483000
H	4.729976000	-1.436942000	-2.065449000
H	5.570762000	0.038675000	-1.572006000
H	6.331626000	-1.545160000	-1.307256000

C	1.541867000	-2.161243000	-2.374286000
H	2.039657000	-1.186998000	-2.277654000
C	1.822567000	-1.882728000	2.790801000
H	2.626038000	-1.199515000	2.484523000
C	2.580082000	-3.180655000	-2.887024000
H	3.061638000	-2.796306000	-3.798268000
H	3.364978000	-3.392906000	-2.154454000
H	2.105648000	-4.137019000	-3.148968000
C	0.451750000	-2.017836000	-3.440548000
H	-0.250885000	-1.223193000	-3.184333000
H	0.909382000	-1.767752000	-4.408958000
H	-0.114578000	-2.949772000	-3.580581000
C	2.441038000	-2.920712000	3.742585000
H	3.038616000	-2.405229000	4.508335000
H	1.674600000	-3.499817000	4.277894000
H	3.096759000	-3.632930000	3.225547000
C	0.813632000	-1.030681000	3.568799000
H	0.425461000	-0.222139000	2.944207000
H	-0.030675000	-1.638108000	3.925042000
H	1.299251000	-0.584925000	4.449974000
C	-0.205805000	-5.906713000	0.457636000
H	-0.525972000	-6.174004000	-0.563084000
C	0.923924000	-6.877159000	0.841003000
H	0.570623000	-7.918063000	0.799428000
H	1.778219000	-6.779569000	0.157179000
H	1.288658000	-6.688423000	1.860580000
C	-1.426139000	-6.088978000	1.370486000
H	-1.194243000	-5.856942000	2.419305000
H	-2.260907000	-5.446939000	1.058669000
H	-1.775846000	-7.131034000	1.335488000
C	0.787380000	3.095692000	-2.576132000
H	1.661113000	2.496109000	-2.290038000
C	0.388097000	3.419593000	2.573616000
H	1.218071000	2.702366000	2.522760000
C	0.943410000	4.751744000	3.114769000
H	1.481735000	4.587325000	4.060086000
H	1.631764000	5.230006000	2.409138000
H	0.133567000	5.466366000	3.319855000
C	-0.629451000	2.871344000	3.585804000
H	-0.967350000	1.861402000	3.334924000
H	-0.170930000	2.821300000	4.584520000
H	-1.516417000	3.515286000	3.668535000
C	1.299060000	4.332657000	-3.335419000
H	1.974630000	4.026447000	-4.148013000
H	0.476940000	4.898772000	-3.795683000
H	1.845589000	5.020966000	-2.678876000
C	-0.063299000	2.227594000	-3.511311000
H	-0.344132000	1.291102000	-3.021757000
H	-0.981489000	2.745569000	-3.824669000
H	0.502743000	1.977167000	-4.421110000
C	-2.839597000	5.871361000	-0.445769000

H	-3.006139000	5.979945000	-1.530492000
C	-2.517090000	7.271398000	0.098816000
H	-1.604741000	7.674558000	-0.362129000
H	-3.341538000	7.968962000	-0.111033000
H	-2.363071000	7.257637000	1.187098000
C	-4.140394000	5.318645000	0.154518000
H	-4.386474000	4.335895000	-0.271028000
H	-4.066297000	5.200818000	1.244889000
H	-4.981279000	5.997992000	-0.049355000

Sum of electronic and thermal Energies= -3131.568622
Sum of electronic and thermal Enthalpies= -3131.567678
Sum of electronic and thermal Free Energies= -3131.711462
Lowest vibration frequencies (/cm^-1) : 23.9305 25.7689 27.5651

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Fe	-0.046975000	-0.976054000	-0.259292000
C	-1.348181000	-3.542539000	0.124108000
C	1.211131000	-3.588490000	-0.142648000
C	-0.059890000	-4.108000000	0.168993000
H	-0.062891000	-5.187410000	0.322903000
N	-1.595782000	-2.222262000	-0.027802000
N	1.467825000	-2.277359000	-0.341547000
C	2.766759000	-1.898359000	-0.814814000
C	2.994045000	-1.763550000	-2.216522000
C	3.832811000	-1.650052000	0.100173000
C	4.254389000	-1.336513000	-2.661216000
C	5.071771000	-1.231416000	-0.407054000
C	5.288944000	-1.061460000	-1.771853000
H	4.435343000	-1.234198000	-3.732216000
H	5.890984000	-1.039952000	0.287118000
H	6.262106000	-0.731686000	-2.139795000
C	-2.958795000	-1.816319000	-0.190941000
C	-3.779648000	-1.556258000	0.948206000
C	-3.501993000	-1.675653000	-1.501965000
C	-5.119033000	-1.191332000	0.741631000
C	-4.845689000	-1.295699000	-1.642511000
C	-5.658672000	-1.062606000	-0.536266000
H	-5.757408000	-1.006718000	1.606402000
H	-5.268942000	-1.195372000	-2.643022000
H	-6.705791000	-0.784184000	-0.668382000
C	1.944461000	-2.132670000	-3.261782000
H	1.015076000	-2.367830000	-2.725696000
C	3.704716000	-1.862087000	1.606172000
H	2.658384000	-2.126872000	1.809098000
C	-3.270975000	-1.666173000	2.382993000
H	-2.189557000	-1.848131000	2.330200000
C	-2.686042000	-1.943282000	-2.761729000
H	-1.667495000	-2.198801000	-2.439256000
P	0.065607000	1.197540000	0.465064000
C	1.611861000	2.114853000	-0.004888000
C	2.454736000	2.752295000	0.920580000

C	1.942596000	2.186343000	-1.370568000
C	3.596935000	3.436625000	0.490545000
H	2.219794000	2.723458000	1.983157000
C	3.078125000	2.875312000	-1.799356000
H	1.295356000	1.712629000	-2.108283000
C	3.912817000	3.502353000	-0.868572000
H	4.239456000	3.923136000	1.226816000
H	3.313035000	2.917701000	-2.864165000
H	4.803754000	4.037156000	-1.201666000
C	-1.218763000	2.408289000	-0.141630000
C	-0.917555000	3.747697000	-0.453898000
C	-2.545723000	1.969788000	-0.293149000
C	-1.915642000	4.617679000	-0.903557000
H	0.100350000	4.119299000	-0.348824000
C	-3.542715000	2.842315000	-0.739558000
H	-2.806802000	0.939140000	-0.064221000
C	-3.231458000	4.169436000	-1.048651000
H	-1.659041000	5.651948000	-1.140997000
H	-4.563436000	2.473977000	-0.850384000
H	-4.008124000	4.849132000	-1.403619000
C	-0.009760000	1.443002000	2.306046000
C	-0.455606000	2.632547000	2.910388000
C	0.399475000	0.382743000	3.132327000
C	-0.475503000	2.758613000	4.302652000
H	-0.793698000	3.464342000	2.294105000
C	0.387212000	0.512236000	4.523954000
H	0.729623000	-0.551708000	2.678168000
C	-0.050160000	1.702095000	5.113954000
H	-0.827141000	3.688287000	4.753992000
H	0.713457000	-0.322209000	5.147313000
H	-0.066653000	1.803141000	6.200495000
C	2.286702000	-4.649112000	-0.295364000
H	3.259782000	-4.236383000	-0.572516000
H	2.402719000	-5.208961000	0.643576000
H	1.995093000	-5.378801000	-1.063759000
C	-2.467319000	-4.568204000	0.178926000
H	-3.462743000	-4.123476000	0.250528000
H	-2.446762000	-5.198334000	-0.722278000
H	-2.324248000	-5.240139000	1.036399000
C	-2.588610000	-0.702358000	-3.662268000
H	-3.572386000	-0.398466000	-4.046923000
H	-2.165944000	0.155729000	-3.123637000
H	-1.947828000	-0.908735000	-4.531512000
C	-3.219470000	-3.147426000	-3.554686000
H	-4.224458000	-2.956462000	-3.957793000
H	-2.558349000	-3.367570000	-4.406204000
H	-3.277056000	-4.048081000	-2.930687000
C	1.634332000	-0.988393000	-4.237001000
H	1.285280000	-0.091904000	-3.710452000
H	2.512639000	-0.703414000	-4.832820000
H	0.847414000	-1.291433000	-4.942619000

C	2.347683000	-3.396594000	-4.040237000
H	3.253651000	-3.227558000	-4.639750000
H	2.547757000	-4.239302000	-3.367717000
H	1.543446000	-3.696173000	-4.728995000
C	4.031557000	-0.593843000	2.408232000
H	3.835683000	-0.758061000	3.478094000
H	5.090177000	-0.314080000	2.311051000
H	3.431674000	0.258764000	2.077265000
C	4.585089000	-3.020847000	2.106597000
H	5.653516000	-2.791994000	1.983805000
H	4.407725000	-3.196379000	3.178385000
H	4.384860000	-3.958088000	1.575397000
C	-3.906418000	-2.839284000	3.148449000
H	-3.732477000	-3.802401000	2.655736000
H	-3.484002000	-2.900624000	4.162518000
H	-4.993478000	-2.708894000	3.252119000
C	-3.484899000	-0.364991000	3.171913000
H	-3.007574000	-0.438890000	4.158890000
H	-3.052751000	0.499867000	2.657752000
H	-4.551696000	-0.159717000	3.339888000

Sum of electronic and thermal Energies= -3537.757852
Sum of electronic and thermal Enthalpies= -3537.756908
Sum of electronic and thermal Free Energies= -3537.904802
Lowest vibration frequencies (/cm^-1) : 9.7925 14.5316 19.3022

^{2}9

Fe	-0.016133000	-1.031232000	-0.214824000
C	-1.356009000	-3.594871000	-0.009950000
C	1.182950000	-3.668977000	-0.180742000
C	-0.093730000	-4.208742000	0.040602000
H	-0.118771000	-5.294113000	0.135415000
N	-1.527140000	-2.257007000	-0.080365000
N	1.412942000	-2.345370000	-0.330801000
C	2.699480000	-1.936365000	-0.812425000
C	2.927518000	-1.859886000	-2.220537000
C	3.761359000	-1.640704000	0.093962000
C	4.190470000	-1.458371000	-2.679996000
C	5.003014000	-1.251167000	-0.429339000
C	5.225604000	-1.151385000	-1.800324000
H	4.374267000	-1.404119000	-3.754142000
H	5.821312000	-1.029973000	0.256914000
H	6.202741000	-0.848197000	-2.180555000
C	-2.866460000	-1.758457000	-0.156539000
C	-3.647235000	-1.606000000	1.031356000
C	-3.435122000	-1.445358000	-1.425790000
C	-4.972739000	-1.162195000	0.907504000
C	-4.763580000	-0.998732000	-1.480947000
C	-5.536602000	-0.861277000	-0.330948000
H	-5.583176000	-1.058901000	1.805586000
H	-5.207394000	-0.767682000	-2.450137000
H	-6.573232000	-0.525978000	-0.398212000

C	1.873402000	-2.256333000	-3.251307000
H	0.948856000	-2.484252000	-2.705095000
C	3.625409000	-1.777925000	1.607347000
H	2.572479000	-2.011978000	1.815850000
C	-3.118536000	-1.925031000	2.428243000
H	-2.046515000	-2.143134000	2.330410000
C	-2.669098000	-1.614154000	-2.732650000
H	-1.652168000	-1.936900000	-2.470872000
P	0.100271000	1.152102000	0.463348000
C	1.662935000	2.084076000	0.073887000
C	2.262434000	2.993996000	0.963072000
C	2.251424000	1.898586000	-1.189280000
C	3.410549000	3.700688000	0.592204000
H	1.837045000	3.154184000	1.951896000
C	3.389634000	2.616237000	-1.564413000
H	1.817797000	1.180666000	-1.882960000
C	3.974752000	3.520808000	-0.673683000
H	3.862653000	4.398402000	1.299678000
H	3.827300000	2.452873000	-2.550181000
H	4.869707000	4.075188000	-0.961206000
C	-1.174776000	2.314167000	-0.243908000
C	-0.841219000	3.430408000	-1.032260000
C	-2.535765000	2.056555000	0.005773000
C	-1.838941000	4.263231000	-1.549719000
H	0.201365000	3.662684000	-1.240065000
C	-3.528935000	2.896812000	-0.502394000
H	-2.827012000	1.191589000	0.596910000
C	-3.185852000	4.004289000	-1.283877000
H	-1.554865000	5.123895000	-2.158286000
H	-4.575651000	2.674153000	-0.291217000
H	-3.962430000	4.657856000	-1.684926000
C	-0.080505000	1.471071000	2.285849000
C	-0.633571000	2.651171000	2.816502000
C	0.389418000	0.490134000	3.175565000
C	-0.701205000	2.844494000	4.200038000
H	-1.011469000	3.424237000	2.148361000
C	0.334548000	0.690493000	4.557448000
H	0.798703000	-0.438188000	2.777416000
C	-0.211436000	1.869341000	5.074412000
H	-1.135930000	3.764971000	4.594325000
H	0.711164000	-0.081164000	5.231243000
H	-0.262239000	2.024514000	6.153452000
C	2.292799000	-4.698672000	-0.279178000
H	3.248294000	-4.272678000	-0.595018000
H	2.440341000	-5.186497000	0.695442000
H	2.019865000	-5.490577000	-0.989949000
C	-2.521413000	-4.563434000	-0.088726000
H	-3.496767000	-4.087217000	0.036795000
H	-2.520655000	-5.064200000	-1.068428000
H	-2.416642000	-5.351848000	0.668628000
C	-2.548158000	-0.295855000	-3.512196000

H	-3.529525000	0.084460000	-3.828609000
H	-2.069391000	0.485671000	-2.910006000
H	-1.947215000	-0.444777000	-4.420705000
C	-3.278264000	-2.712045000	-3.620035000
H	-4.291680000	-2.447087000	-3.954069000
H	-2.662204000	-2.861161000	-4.519283000
H	-3.342822000	-3.671555000	-3.091945000
C	1.551808000	-1.129578000	-4.244202000
H	1.183822000	-0.230787000	-3.733718000
H	2.428298000	-0.841167000	-4.841240000
H	0.771767000	-1.454845000	-4.947735000
C	2.276183000	-3.531349000	-4.011649000
H	3.171233000	-3.368050000	-4.628926000
H	2.492034000	-4.359887000	-3.326637000
H	1.463613000	-3.849357000	-4.681872000
C	3.979958000	-0.480578000	2.349601000
H	3.773026000	-0.589458000	3.424372000
H	5.046855000	-0.235896000	2.249908000
H	3.407464000	0.373584000	1.976057000
C	4.479097000	-2.930096000	2.165710000
H	5.552251000	-2.732926000	2.029836000
H	4.299899000	-3.046249000	3.245230000
H	4.254729000	-3.887617000	1.683289000
C	-3.794730000	-3.159952000	3.048723000
H	-3.685352000	-4.054423000	2.426719000
H	-3.350070000	-3.378691000	4.031006000
H	-4.870071000	-2.990400000	3.204217000
C	-3.265507000	-0.736309000	3.390835000
H	-2.784844000	-0.968982000	4.351436000
H	-2.796226000	0.170996000	2.997884000
H	-4.320157000	-0.509370000	3.602291000

Sum of electronic and thermal Energies= -3537.719151
Sum of electronic and thermal Enthalpies= -3537.718207
Sum of electronic and thermal Free Energies= -3537.863451
Lowest vibration frequencies (/cm^-1) : 13.6120 23.1542 26.1070

[4]9'

Fe	-0.162123000	-1.014198000	-0.674801000
C	-1.397912000	-3.540712000	0.005816000
C	1.103499000	-3.553290000	-0.057753000
C	-0.145592000	-4.154789000	0.112350000
H	-0.145062000	-5.216150000	0.333962000
N	-1.624546000	-2.271787000	-0.291645000
N	1.329052000	-2.276579000	-0.336785000
H	-2.274145000	-4.174288000	0.172037000
H	1.977215000	-4.203185000	0.037862000
C	2.666046000	-1.818451000	-0.420905000
C	3.070030000	-1.176030000	-1.613875000
C	3.555632000	-1.912921000	0.670630000
C	4.352658000	-0.641090000	-1.699503000
C	4.833031000	-1.354313000	0.543489000

C	5.235155000	-0.723673000	-0.626039000
H	4.655914000	-0.146472000	-2.614117000
H	5.513241000	-1.414852000	1.385675000
H	6.225949000	-0.294081000	-0.701517000
C	-2.963287000	-1.810750000	-0.327834000
C	-3.609280000	-1.461658000	0.874825000
C	-3.587182000	-1.604527000	-1.573150000
C	-4.897080000	-0.924192000	0.808899000
C	-4.875138000	-1.063792000	-1.597173000
C	-5.530978000	-0.728530000	-0.415494000
H	-5.397810000	-0.646498000	1.728775000
H	-5.362029000	-0.905004000	-2.552222000
H	-6.529998000	-0.312161000	-0.448591000
C	2.123557000	-1.073862000	-2.777118000
H	1.618295000	-2.022077000	-2.970358000
H	1.348966000	-0.314073000	-2.597620000
H	2.651568000	-0.768563000	-3.681627000
C	3.175121000	-2.574276000	1.969870000
H	2.095751000	-2.607637000	2.115653000
H	3.530457000	-3.608226000	2.014775000
H	3.619778000	-2.041000000	2.812897000
C	-2.887387000	-1.611440000	2.182105000
H	-2.676649000	-2.657984000	2.415770000
H	-1.920301000	-1.101324000	2.144921000
H	-3.469473000	-1.189457000	3.001739000
C	-2.852018000	-1.932812000	-2.840991000
H	-1.963596000	-1.299498000	-2.954223000
H	-2.497521000	-2.965481000	-2.845482000
H	-3.486342000	-1.778976000	-3.714468000
P	0.005595000	1.116391000	0.042132000
C	1.550366000	1.951800000	-0.490343000
C	2.662273000	2.072081000	0.350108000
C	1.658570000	2.374243000	-1.824515000
C	3.853526000	2.612530000	-0.130695000
H	2.601621000	1.737052000	1.376796000
C	2.847298000	2.918834000	-2.299386000
H	0.805405000	2.285765000	-2.487723000
C	3.949346000	3.038858000	-1.452268000
H	4.708057000	2.689599000	0.528805000
H	2.914317000	3.246900000	-3.329063000
H	4.876546000	3.456233000	-1.823536000
C	-1.295671000	2.338879000	-0.361428000
C	-1.053584000	3.716301000	-0.458946000
C	-2.598440000	1.858894000	-0.550983000
C	-2.098260000	4.594139000	-0.740706000
H	-0.049201000	4.097713000	-0.324382000
C	-3.641790000	2.739865000	-0.825882000
H	-2.795896000	0.795987000	-0.481536000
C	-3.393018000	4.107851000	-0.922922000
H	-1.901266000	5.655980000	-0.817721000
H	-4.640854000	2.349119000	-0.967689000

H	-4.202254000	4.792675000	-1.142643000
C	0.091478000	1.171709000	1.872149000
C	-0.444875000	2.205847000	2.647467000
C	0.710722000	0.088747000	2.511648000
C	-0.355484000	2.156524000	4.037907000
H	-0.941804000	3.039711000	2.169172000
C	0.808538000	0.047143000	3.899416000
H	1.103543000	-0.719151000	1.906131000
C	0.273006000	1.081999000	4.665697000
H	-0.779582000	2.957390000	4.630207000
H	1.291049000	-0.795205000	4.378711000
H	0.338569000	1.048252000	5.745705000

Sum of electronic and thermal Energies= -2003.270931
Sum of electronic and thermal Enthalpies= -2003.269987
Sum of electronic and thermal Free Energies= -2003.384836
Lowest vibration frequencies (/cm^-1) : 16.2081 20.7596 23.9843

^{2}9'

Fe	-0.548908000	-0.990044000	-0.092479000
C	-1.930525000	-3.569732000	-0.018169000
C	0.533916000	-3.708262000	-0.060428000
C	-0.734448000	-4.287916000	-0.050183000
H	-0.791146000	-5.369997000	-0.041944000
N	-2.004571000	-2.254377000	-0.030875000
N	0.818340000	-2.414587000	-0.072737000
H	-2.869028000	-4.129217000	0.027864000
H	1.385549000	-4.395191000	-0.051926000
C	2.195994000	-2.076658000	-0.014883000
C	2.867997000	-1.726471000	-1.200568000
C	2.860366000	-2.064529000	1.225881000
C	4.198064000	-1.311793000	-1.119911000
C	4.192275000	-1.640765000	1.267445000
C	4.856160000	-1.258075000	0.105626000
H	4.714304000	-1.019533000	-2.026313000
H	4.707328000	-1.615022000	2.221143000
H	5.884428000	-0.922219000	0.153716000
C	-3.279751000	-1.631728000	0.009745000
C	-3.784077000	-1.177193000	1.244229000
C	-3.962379000	-1.375264000	-1.194930000
C	-4.998153000	-0.485598000	1.255308000
C	-5.173425000	-0.681124000	-1.142255000
C	-5.692635000	-0.242159000	0.073069000
H	-5.395944000	-0.135440000	2.200294000
H	-5.705670000	-0.479703000	-2.064384000
H	-6.634010000	0.292373000	0.098655000
C	2.151180000	-1.830443000	-2.513625000
H	1.960442000	-2.874998000	-2.776893000
H	1.173908000	-1.343134000	-2.456547000
H	2.728779000	-1.370494000	-3.315315000
C	2.140715000	-2.505184000	2.470926000
H	1.128065000	-2.094888000	2.508337000

H	2.032186000	-3.592885000	2.506068000
H	2.681013000	-2.195575000	3.367326000
C	-3.000841000	-1.411605000	2.503867000
H	-2.814227000	-2.474905000	2.669684000
H	-2.016258000	-0.932934000	2.444277000
H	-3.524381000	-1.011378000	3.372386000
C	-3.362217000	-1.814657000	-2.498883000
H	-2.336651000	-1.443774000	-2.596165000
H	-3.299724000	-2.903247000	-2.570211000
H	-3.946139000	-1.448336000	-3.343532000
P	0.377549000	1.079300000	-0.037854000
C	1.872084000	1.567328000	-0.982000000
C	3.047715000	2.019399000	-0.374829000
C	1.835394000	1.439022000	-2.378374000
C	4.165109000	2.330769000	-1.148560000
H	3.097016000	2.123899000	0.700261000
C	2.947647000	1.759295000	-3.148543000
H	0.929867000	1.091524000	-2.861624000
C	4.119546000	2.202525000	-2.533642000
H	5.070953000	2.671199000	-0.663573000
H	2.902125000	1.659513000	-4.225654000
H	4.988234000	2.445681000	-3.132089000
C	-0.887239000	2.243536000	-0.692573000
C	-0.568105000	3.459178000	-1.313598000
C	-2.237876000	1.898836000	-0.536116000
C	-1.578043000	4.303913000	-1.769646000
H	0.469015000	3.738867000	-1.446190000
C	-3.246649000	2.745287000	-0.989902000
H	-2.515543000	0.964403000	-0.058509000
C	-2.917476000	3.949372000	-1.609237000
H	-1.318133000	5.238195000	-2.250941000
H	-4.280142000	2.451395000	-0.863450000
H	-3.698965000	4.606635000	-1.968616000
C	0.710003000	1.758760000	1.634202000
C	0.197025000	2.978791000	2.089476000
C	1.507399000	0.991538000	2.494914000
C	0.480493000	3.421162000	3.381307000
H	-0.426616000	3.579722000	1.440925000
C	1.798487000	1.441200000	3.779144000
H	1.906076000	0.049442000	2.144583000
C	1.282209000	2.657109000	4.226927000
H	0.074228000	4.364186000	3.724455000
H	2.421442000	0.840128000	4.429354000
H	1.500535000	3.004620000	5.228607000

Sum of electronic and thermal Energies= -2003.218538
Sum of electronic and thermal Enthalpies= -2003.217594
Sum of electronic and thermal Free Energies= -2003.329421
Lowest vibration frequencies (/cm^-1) : -14.0677(*) 10.2423 17.7229
(*) corresponds to the rotation of one phenyl group around the P—Ph bond of the PPh_3 moiety

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Fe	-0.800382000	-1.570470000	-0.075780000
N	1.069518000	-1.548337000	0.339977000
N	-2.679615000	-1.553841000	-0.445174000
Si	1.538063000	-0.218686000	1.348509000
Si	2.007476000	-2.888630000	-0.225109000
Si	-3.156444000	-0.741426000	-1.898132000
Si	-3.651089000	-2.395780000	0.716235000
C	3.120075000	-3.664321000	1.132879000
H	2.506488000	-4.034569000	1.967753000
H	3.692495000	-4.517266000	0.734801000
H	3.841645000	-2.946453000	1.547668000
C	3.172989000	-2.425118000	-1.674098000
H	2.591493000	-2.014700000	-2.513045000
H	3.910549000	-1.664210000	-1.382474000
H	3.725780000	-3.303017000	-2.045416000
C	3.343477000	0.370293000	1.052082000
H	4.088534000	-0.415667000	1.240236000
H	3.480878000	0.716126000	0.016874000
H	3.582245000	1.215342000	1.717301000
C	1.429504000	-0.614408000	3.219082000
H	1.718542000	0.251736000	3.836047000
H	0.402794000	-0.897483000	3.491825000
H	2.084965000	-1.454582000	3.491208000
C	0.495617000	1.357752000	1.071776000
H	0.524979000	1.663460000	0.015887000
H	-0.559415000	1.201891000	1.336393000
H	0.884454000	2.192656000	1.680000000
C	-1.732361000	-0.494330000	-3.146437000
H	-2.106490000	-0.011474000	-4.065881000
H	-0.930703000	0.132765000	-2.731946000
H	-1.279972000	-1.456407000	-3.426788000
C	-4.030072000	-4.202203000	0.204513000
H	-4.630834000	-4.725155000	0.965963000
H	-4.580106000	-4.246599000	-0.746520000
H	-3.093764000	-4.762873000	0.068521000
C	-5.354994000	-1.566305000	1.030942000
H	-5.932896000	-2.140924000	1.772126000
H	-5.224187000	-0.549258000	1.429602000
H	-5.968887000	-1.489184000	0.122680000
C	-4.496648000	-1.687645000	-2.896636000
H	-4.127544000	-2.680462000	-3.194421000
H	-5.425420000	-1.838624000	-2.328321000
H	-4.757753000	-1.140396000	-3.816420000
C	-3.867317000	1.007479000	-1.573056000
H	-4.776439000	0.970319000	-0.956006000
H	-3.130050000	1.621576000	-1.035251000
H	-4.118497000	1.525855000	-2.512314000
C	-2.865618000	-2.493699000	2.454218000
H	-1.920280000	-3.053758000	2.444820000
H	-2.644600000	-1.487848000	2.839498000
H	-3.552594000	-2.987579000	3.163090000

C	0.956819000	-4.346729000	-0.869440000
H	0.282847000	-4.725316000	-0.087746000
H	0.330126000	-4.050423000	-1.722218000
H	1.607460000	-5.177650000	-1.193174000

Sum of electronic and thermal Energies= -3009.711572
Sum of electronic and thermal Enthalpies= -3009.710627
Sum of electronic and thermal Free Energies= -3009.817988
Lowest vibration frequencies (/cm^-1) : 13.4739 20.6315 26.2646

^{2}10

Fe	-0.797145000	-1.582618000	-0.040487000
N	1.063147000	-1.526519000	0.279019000
N	-2.665644000	-1.585546000	-0.401868000
Si	1.513594000	-0.136675000	1.217607000
Si	1.982331000	-2.918770000	-0.189488000
Si	-3.141792000	-0.686433000	-1.803121000
Si	-3.622667000	-2.507174000	0.708766000
C	2.967394000	-3.696242000	1.261730000
H	2.281735000	-4.022379000	2.058025000
H	3.536019000	-4.578803000	0.928058000
H	3.681368000	-2.991634000	1.711278000
C	3.255604000	-2.519751000	-1.565531000
H	2.744128000	-2.094111000	-2.441832000
H	4.008838000	-1.790044000	-1.237717000
H	3.787456000	-3.426503000	-1.895323000
C	3.362278000	0.351320000	1.005450000
H	4.054767000	-0.452411000	1.293822000
H	3.584880000	0.622869000	-0.037127000
H	3.597646000	1.227072000	1.631027000
C	1.274138000	-0.396959000	3.098268000
H	1.556770000	0.500424000	3.671943000
H	0.223741000	-0.629391000	3.323108000
H	1.882852000	-1.236531000	3.464808000
C	0.576379000	1.462617000	0.758003000
H	0.674814000	1.676333000	-0.316222000
H	-0.496221000	1.378714000	0.978332000
H	0.980244000	2.325437000	1.315372000
C	-1.725711000	-0.406338000	-3.053394000
H	-2.099336000	0.117819000	-3.950025000
H	-0.911511000	0.190761000	-2.620488000
H	-1.290978000	-1.363575000	-3.375616000
C	-3.988150000	-4.283181000	0.091230000
H	-4.588796000	-4.852446000	0.818815000
H	-4.534243000	-4.274786000	-0.863084000
H	-3.048537000	-4.830366000	-0.073103000
C	-5.332085000	-1.710955000	1.075562000
H	-5.900117000	-2.324105000	1.793130000
H	-5.207485000	-0.711736000	1.518822000
H	-5.952280000	-1.597948000	0.175408000
C	-4.508458000	-1.551258000	-2.841573000
H	-4.161121000	-2.531960000	-3.199788000

H	-5.436967000	-1.716599000	-2.276886000
H	-4.763694000	-0.946706000	-3.726464000
C	-3.821140000	1.051380000	-1.373712000
H	-4.719328000	0.990952000	-0.742356000
H	-3.066362000	1.627000000	-0.818499000
H	-4.084022000	1.621993000	-2.278814000
C	-2.828003000	-2.701037000	2.434532000
H	-1.870870000	-3.238447000	2.385939000
H	-2.626270000	-1.716865000	2.881375000
H	-3.500504000	-3.253237000	3.113443000
C	0.935625000	-4.353489000	-0.887149000
H	0.211950000	-4.716566000	-0.144179000
H	0.362228000	-4.042529000	-1.771469000
H	1.584354000	-5.198624000	-1.176855000

Sum of electronic and thermal Energies= -3009.662320
Sum of electronic and thermal Enthalpies= -3009.661376
Sum of electronic and thermal Free Energies= -3009.767805
Lowest vibration frequencies (/cm^-1) : 19.1938 25.9383 28.0288

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Fe	-0.727935000	-1.527821000	0.318334000
N	1.067652000	-1.247726000	0.914255000
Si	1.908360000	-2.708000000	1.440157000
C	3.595098000	-2.372231000	2.249085000
H	3.493639000	-1.875540000	3.222131000
H	4.117236000	-3.326317000	2.416370000
H	4.241445000	-1.741099000	1.627218000
C	2.207741000	-3.907148000	-0.015405000
H	1.298840000	-4.078400000	-0.609750000
H	2.977523000	-3.528279000	-0.701260000
H	2.547845000	-4.886832000	0.354419000
C	1.654770000	0.038240000	1.031872000
C	2.507745000	0.554897000	0.000427000
C	1.414727000	0.866619000	2.177215000
C	3.111682000	1.810525000	0.157952000
C	2.047644000	2.114478000	2.280333000
C	2.902472000	2.591978000	1.291141000
H	3.765552000	2.186943000	-0.631128000
H	1.871246000	2.727692000	3.166158000
H	3.391623000	3.562027000	1.397817000
C	-4.326148000	-1.650630000	-1.888198000
C	-4.671770000	-2.464636000	-0.860796000
H	-4.887246000	-1.317836000	-2.751554000
H	-5.595674000	-2.985437000	-0.647888000
C	-2.485700000	-1.807064000	-0.502579000
C	-3.577492000	-3.437079000	1.110703000
C	-4.081016000	-2.949844000	2.342026000
C	-3.199630000	-4.793515000	0.937595000
C	-4.153201000	-3.848245000	3.417567000
C	-3.293130000	-5.640725000	2.052449000
C	-3.756417000	-5.176172000	3.281222000

H	-4.533780000	-3.503225000	4.378513000
H	-3.009018000	-6.688015000	1.953507000
H	-3.819713000	-5.855384000	4.133039000
C	-2.350531000	-0.399934000	-2.614391000
C	-2.441061000	1.003415000	-2.446420000
C	-1.752161000	-0.985311000	-3.757501000
C	-1.907626000	1.813806000	-3.460673000
C	-1.238906000	-0.121569000	-4.736247000
C	-1.316453000	1.262296000	-4.594958000
H	-1.965385000	2.897834000	-3.364289000
H	-0.774912000	-0.540060000	-5.629474000
H	-0.913755000	1.913979000	-5.372124000
N	-3.564831000	-2.563493000	-0.031769000
N	-3.014451000	-1.258419000	-1.670903000
C	0.864837000	-3.667361000	2.715556000
H	0.733699000	-3.086579000	3.639084000
H	-0.139364000	-3.921471000	2.348729000
H	1.362207000	-4.612325000	2.985371000
C	2.761468000	-0.204989000	-1.294824000
H	2.186627000	-1.137366000	-1.222511000
C	0.481250000	0.447854000	3.306120000
H	0.046400000	-0.518624000	3.011274000
C	4.238389000	-0.571780000	-1.504094000
H	4.358283000	-1.177162000	-2.415786000
H	4.867786000	0.322592000	-1.621307000
H	4.640742000	-1.149049000	-0.662776000
C	2.231532000	0.566354000	-2.512575000
H	2.782130000	1.505105000	-2.671453000
H	2.337475000	-0.035727000	-3.427622000
H	1.171105000	0.817774000	-2.394944000
C	1.217040000	0.239495000	4.638775000
H	2.025097000	-0.495358000	4.542427000
H	1.663680000	1.174892000	5.005932000
H	0.522038000	-0.120773000	5.412934000
C	-0.673042000	1.445022000	3.489625000
H	-0.309129000	2.445022000	3.764923000
H	-1.261058000	1.551110000	2.568501000
H	-1.349958000	1.113853000	4.290274000
C	-1.679189000	-2.491893000	-3.968928000
H	-2.096037000	-2.969700000	-3.073971000
C	-3.124653000	1.647706000	-1.248002000
H	-3.337386000	0.852236000	-0.521829000
C	-4.589907000	-1.524784000	2.514419000
H	-4.244321000	-0.944028000	1.648874000
C	-2.774976000	-5.365490000	-0.409560000
H	-2.542940000	-4.518469000	-1.067410000
C	-3.927269000	-6.152322000	-1.058456000
H	-4.823228000	-5.532342000	-1.190903000
H	-3.625434000	-6.522202000	-2.049424000
H	-4.209620000	-7.021729000	-0.447706000
C	-1.511383000	-6.233774000	-0.332551000

H	-1.686106000	-7.177293000	0.202602000
H	-1.178764000	-6.496657000	-1.347011000
H	-0.688703000	-5.709712000	0.167177000
C	-6.127737000	-1.481288000	2.517225000
H	-6.540330000	-2.044172000	3.366621000
H	-6.479204000	-0.442440000	2.600676000
H	-6.551968000	-1.905940000	1.598154000
C	-4.029405000	-0.842419000	3.769090000
H	-4.296910000	0.223563000	3.767400000
H	-4.433957000	-1.275891000	4.694325000
H	-2.936589000	-0.917960000	3.808677000
C	-2.536887000	-2.939583000	-5.163543000
H	-2.163509000	-2.526591000	-6.111191000
H	-2.524219000	-4.035822000	-5.251732000
H	-3.582998000	-2.623315000	-5.051715000
C	-0.232660000	-2.989430000	-4.105086000
H	0.370224000	-2.695650000	-3.236863000
H	-0.216003000	-4.086944000	-4.175691000
H	0.256795000	-2.595098000	-5.006442000
C	-4.470789000	2.277187000	-1.643536000
H	-4.335534000	3.102373000	-2.357079000
H	-5.142469000	1.541657000	-2.106315000
H	-4.977090000	2.683786000	-0.755744000
C	-2.225220000	2.671591000	-0.539524000
H	-2.024126000	3.551689000	-1.165857000
H	-2.716235000	3.031153000	0.376113000
H	-1.259002000	2.235114000	-0.256415000

Sum of electronic and thermal Energies= -3353.755824
Sum of electronic and thermal Enthalpies= -3353.754880
Sum of electronic and thermal Free Energies= -3353.906511
Lowest vibration frequencies (/cm^-1) : 14.3773 22.3194 25.5295

^{2}11

Fe	-0.732817000	-1.552548000	0.344061000
N	1.069197000	-1.267023000	0.863983000
Si	1.911540000	-2.734649000	1.377820000
C	3.612350000	-2.399690000	2.159467000
H	3.521015000	-1.932729000	3.148389000
H	4.147965000	-3.352007000	2.290525000
H	4.240828000	-1.743273000	1.546104000
C	2.177356000	-3.924382000	-0.089930000
H	1.247267000	-4.115433000	-0.643565000
H	2.907207000	-3.524878000	-0.807296000
H	2.556374000	-4.896110000	0.262475000
C	1.644095000	0.019594000	1.010800000
C	2.494702000	0.559781000	-0.011270000
C	1.400941000	0.822691000	2.173421000
C	3.091990000	1.814755000	0.171490000
C	2.025161000	2.072490000	2.299679000
C	2.876452000	2.573596000	1.318982000
H	3.744491000	2.210174000	-0.609274000

H	1.846628000	2.667992000	3.197088000
H	3.358681000	3.544918000	1.443611000
C	-4.297020000	-1.635802000	-1.883785000
C	-4.649424000	-2.464555000	-0.871115000
H	-4.850050000	-1.294509000	-2.748970000
H	-5.573080000	-2.992080000	-0.674260000
C	-2.468449000	-1.797748000	-0.478898000
C	-3.587776000	-3.423881000	1.122815000
C	-4.127238000	-2.920261000	2.332433000
C	-3.197223000	-4.780587000	0.982708000
C	-4.217809000	-3.800531000	3.421813000
C	-3.309608000	-5.608706000	2.109876000
C	-3.805433000	-5.126475000	3.319227000
H	-4.625749000	-3.442484000	4.366684000
H	-3.014105000	-6.654918000	2.036801000
H	-3.882893000	-5.790923000	4.181470000
C	-2.321247000	-0.383240000	-2.589301000
C	-2.411842000	1.020443000	-2.426707000
C	-1.727499000	-0.972329000	-3.733150000
C	-1.885874000	1.827460000	-3.447352000
C	-1.221345000	-0.111874000	-4.718551000
C	-1.301589000	1.272291000	-4.583505000
H	-1.943941000	2.911845000	-3.354584000
H	-0.761555000	-0.533405000	-5.612535000
H	-0.905569000	1.921413000	-5.366251000
N	-3.551026000	-2.567028000	-0.031597000
N	-2.989566000	-1.239290000	-1.646192000
C	0.904943000	-3.696538000	2.681422000
H	0.804516000	-3.120419000	3.611689000
H	-0.109968000	-3.950453000	2.346374000
H	1.414453000	-4.640812000	2.931098000
C	2.753538000	-0.174936000	-1.320154000
H	2.174229000	-1.106085000	-1.270986000
C	0.477582000	0.371571000	3.297535000
H	0.059061000	-0.599155000	2.990716000
C	4.230206000	-0.543999000	-1.528161000
H	4.353552000	-1.122750000	-2.456504000
H	4.865007000	0.350068000	-1.614208000
H	4.623213000	-1.148643000	-0.702057000
C	2.236509000	0.624374000	-2.525282000
H	2.797752000	1.559883000	-2.664091000
H	2.340755000	0.038382000	-3.450819000
H	1.178478000	0.883773000	-2.406829000
C	1.221133000	0.157949000	4.625003000
H	2.051693000	-0.549101000	4.512218000
H	1.639190000	1.098737000	5.011365000
H	0.538744000	-0.239597000	5.391959000
C	-0.694312000	1.344584000	3.496294000
H	-0.346851000	2.349298000	3.775499000
H	-1.290233000	1.444985000	2.579634000
H	-1.358956000	0.995657000	4.299632000

C	-1.649016000	-2.479707000	-3.938230000
H	-2.056360000	-2.955787000	-3.038035000
C	-3.088834000	1.668341000	-1.226670000
H	-3.296935000	0.874809000	-0.497046000
C	-4.656135000	-1.498262000	2.467893000
H	-4.298820000	-0.928260000	1.600015000
C	-2.740637000	-5.371777000	-0.345611000
H	-2.471370000	-4.534170000	-1.001495000
C	-3.887368000	-6.141988000	-1.024017000
H	-4.764161000	-5.504716000	-1.195162000
H	-3.559927000	-6.531551000	-1.999187000
H	-4.208494000	-6.996640000	-0.411620000
C	-1.498595000	-6.265282000	-0.224018000
H	-1.712635000	-7.207302000	0.299411000
H	-1.133807000	-6.531825000	-1.226362000
H	-0.684351000	-5.760223000	0.307794000
C	-6.194084000	-1.471717000	2.436079000
H	-6.619719000	-2.027439000	3.283753000
H	-6.557589000	-0.435404000	2.497692000
H	-6.593162000	-1.912510000	1.513549000
C	-4.132951000	-0.787486000	3.722898000
H	-4.409332000	0.275952000	3.694640000
H	-4.557308000	-1.207429000	4.645527000
H	-3.040981000	-0.852325000	3.791900000
C	-2.511978000	-2.938268000	-5.124902000
H	-2.146945000	-2.527659000	-6.076827000
H	-2.493507000	-4.034835000	-5.207843000
H	-3.559076000	-2.627700000	-5.007703000
C	-0.200936000	-2.970375000	-4.083263000
H	0.407709000	-2.668301000	-3.222141000
H	-0.178753000	-4.068248000	-4.147196000
H	0.279121000	-2.579315000	-4.991069000
C	-4.437072000	2.296408000	-1.617133000
H	-4.305950000	3.118755000	-2.334767000
H	-5.111333000	1.559006000	-2.073285000
H	-4.938527000	2.706595000	-0.728228000
C	-2.184887000	2.693709000	-0.526390000
H	-1.984774000	3.570602000	-1.157615000
H	-2.671799000	3.058353000	0.389525000
H	-1.219070000	2.255473000	-0.245142000

Sum of electronic and thermal Energies= -3353.713596
Sum of electronic and thermal Enthalpies= -3353.712652
Sum of electronic and thermal Free Energies= -3353.862816
Lowest vibration frequencies (/cm^-1) : 15.9747 21.9994 25.5142

^{4}11'

Fe	-0.701025000	-1.639143000	0.407208000
N	1.185601000	-1.438914000	0.560442000
Si	2.200599000	-2.797525000	0.095567000
C	3.615510000	-3.053398000	1.336420000
H	3.218057000	-3.241019000	2.344180000

H	4.245313000	-3.910730000	1.055580000
H	4.263923000	-2.168292000	1.399057000
C	2.927566000	-2.700877000	-1.663661000
H	2.148866000	-2.441890000	-2.395859000
H	3.729621000	-1.955635000	-1.756014000
H	3.351825000	-3.673489000	-1.957120000
C	1.600794000	-0.156479000	0.900724000
C	2.711905000	0.509603000	0.321393000
C	0.860324000	0.583109000	1.862995000
C	3.037452000	1.821654000	0.666970000
H	3.307599000	-0.004730000	-0.431529000
C	1.180438000	1.900338000	2.193890000
H	0.043374000	0.075035000	2.386183000
C	2.274557000	2.536748000	1.597955000
H	3.898578000	2.296919000	0.191133000
H	0.580370000	2.425993000	2.940203000
H	2.533155000	3.563554000	1.859683000
C	-4.351693000	-1.663539000	-1.616830000
C	-4.706429000	-2.408135000	-0.539390000
H	-4.937630000	-1.336487000	-2.466039000
H	-5.658962000	-2.848136000	-0.273343000
C	-2.517850000	-1.760435000	-0.229629000
C	-3.571038000	-3.150518000	1.532517000
C	-2.930827000	-2.579184000	2.644479000
C	-4.169026000	-4.415859000	1.648448000
C	-2.880340000	-3.276961000	3.853153000
H	-2.512435000	-1.575368000	2.566857000
C	-4.126364000	-5.096427000	2.866341000
H	-4.636303000	-4.878148000	0.778939000
C	-3.478004000	-4.535253000	3.972000000
H	-2.382243000	-2.822438000	4.710603000
H	-4.587716000	-6.082047000	2.943254000
H	-3.439390000	-5.075160000	4.918650000
C	-2.302786000	-0.472285000	-2.336402000
C	-1.443796000	0.531650000	-1.862366000
C	-2.423206000	-0.694609000	-3.716709000
C	-0.703638000	1.296352000	-2.766814000
H	-1.389167000	0.743669000	-0.794450000
C	-1.692160000	0.088804000	-4.612540000
H	-3.058292000	-1.499887000	-4.086078000
C	-0.825829000	1.081435000	-4.143182000
H	-0.034321000	2.067915000	-2.384971000
H	-1.788109000	-0.094467000	-5.683756000
H	-0.248142000	1.682720000	-4.846181000
N	-3.604054000	-2.454802000	0.302491000
N	-3.037973000	-1.263198000	-1.421555000
C	1.066649000	-4.325156000	0.131907000
H	0.606453000	-4.472884000	1.119891000
H	0.259810000	-4.277600000	-0.615875000
H	1.652836000	-5.229463000	-0.093727000

Sum of electronic and thermal Energies= -2646.991973

Sum of electronic and thermal Enthalpies= -2646.991029
Sum of electronic and thermal Free Energies= -2647.091602
Lowest vibration frequencies (/cm^-1) : 3.2004 10.8811 21.0638

^{2}11'

Fe	-0.417912000	-1.379405000	0.311283000
N	1.283157000	-2.056931000	0.836718000
Si	2.339555000	-3.249527000	0.095098000
C	3.981405000	-3.311874000	1.049281000
H	3.801854000	-3.519071000	2.113752000
H	4.634416000	-4.105868000	0.657237000
H	4.534231000	-2.364080000	0.985727000
C	2.699556000	-2.958693000	-1.753203000
H	1.768106000	-2.899252000	-2.335294000
H	3.260189000	-2.031119000	-1.934122000
H	3.293087000	-3.789258000	-2.165438000
C	1.386998000	-0.702132000	1.027664000
C	2.318589000	0.221634000	0.439417000
C	0.294824000	-0.145423000	1.820086000
C	2.168784000	1.583874000	0.622467000
H	3.155233000	-0.163246000	-0.143229000
C	0.178992000	1.265491000	1.972720000
H	-0.155608000	-0.798806000	2.579619000
C	1.085859000	2.119451000	1.368917000
H	2.901029000	2.264796000	0.182225000
H	-0.615235000	1.666149000	2.606926000
H	0.996958000	3.199505000	1.496249000
C	-4.135538000	-1.413034000	-1.541199000
C	-4.438117000	-2.135553000	-0.432121000
H	-4.753389000	-1.131632000	-2.384191000
H	-5.361557000	-2.615440000	-0.132777000
C	-2.259853000	-1.414711000	-0.192705000
C	-3.274979000	-2.747161000	1.655295000
C	-3.017948000	-1.990064000	2.806521000
C	-3.529377000	-4.121881000	1.759166000
C	-3.005804000	-2.613109000	4.055796000
H	-2.846964000	-0.918996000	2.711477000
C	-3.526324000	-4.733925000	3.015325000
H	-3.708139000	-4.706714000	0.856693000
C	-3.260777000	-3.984782000	4.165094000
H	-2.808325000	-2.019793000	4.949773000
H	-3.719580000	-5.804959000	3.091131000
H	-3.252669000	-4.467216000	5.143294000
C	-2.140109000	-0.200253000	-2.356407000
C	-1.270208000	0.823067000	-1.947703000
C	-2.315873000	-0.461501000	-3.725372000
C	-0.578704000	1.567984000	-2.904877000
H	-1.159296000	1.048016000	-0.887112000
C	-1.632369000	0.303311000	-4.672417000
H	-2.959670000	-1.280313000	-4.046441000
C	-0.757782000	1.317477000	-4.269183000

H	0.096299000	2.357845000	-2.573599000
H	-1.772500000	0.089005000	-5.733049000
H	-0.218754000	1.905832000	-5.012660000
N	-3.319425000	-2.113289000	0.384365000
N	-2.831242000	-0.966827000	-1.389741000
C	1.448046000	-4.911168000	0.268643000
H	1.239824000	-5.133845000	1.324492000
H	0.486148000	-4.904193000	-0.263598000
H	2.053319000	-5.733451000	-0.140921000

Sum of electronic and thermal Energies= -2646.961388
Sum of electronic and thermal Enthalpies= -2646.960444
Sum of electronic and thermal Free Energies= -2647.056137
Lowest vibration frequencies (/cm^-1) : 13.4300 23.7149 26.5447

^{4}12

Fe	0.989030000	0.123744000	0.000200000
C	1.230285000	2.912230000	3.271598000
C	2.145639000	2.005435000	3.741808000
C	2.850588000	-3.747482000	-0.667188000
C	3.941485000	-2.921617000	-0.761854000
C	-3.329205000	-0.086888000	0.435498000
C	-2.925460000	-0.727501000	1.579166000
C	1.705512000	1.255826000	-4.092638000
C	2.278714000	2.352121000	-3.500367000
C	-1.018140000	-0.178095000	0.390888000
C	2.115879000	-1.591561000	-0.261673000
C	1.428058000	1.247671000	1.677464000
C	1.424615000	1.026440000	-1.807829000
C	-0.189190000	3.085256000	1.226537000
H	-0.192963000	2.613363000	0.240652000
H	-1.185029000	2.972738000	1.677182000
H	0.032619000	4.154454000	1.116925000
C	3.093915000	-0.142906000	2.908773000
H	2.902453000	-0.801592000	2.058330000
H	4.155007000	0.142945000	2.921367000
H	2.866291000	-0.679886000	3.839556000
C	2.602883000	3.128636000	-1.156132000
H	2.415554000	2.713899000	-0.162840000
H	3.683349000	3.278022000	-1.286293000
H	2.102343000	4.102577000	-1.249394000
C	0.552734000	-0.795504000	-3.261342000
H	1.278104000	-1.556174000	-3.581824000
H	0.111654000	-1.106749000	-2.311211000
H	-0.236255000	-0.714382000	-4.020051000
C	4.315971000	-0.463978000	-0.559283000
H	5.217715000	-0.609380000	0.049352000
H	4.616334000	-0.237590000	-1.591727000
H	3.745709000	0.380132000	-0.164367000
C	0.421771000	-3.425236000	-0.222486000
H	0.340196000	-4.094136000	0.645624000
H	-0.240806000	-2.567283000	-0.087116000

H	0.114752000	-3.979306000	-1.119918000
C	-0.720455000	-1.340394000	2.572417000
H	0.309330000	-1.389093000	2.209898000
H	-0.749943000	-0.717522000	3.477177000
H	-1.064801000	-2.351278000	2.826165000
C	-2.172993000	0.946985000	-1.513839000
H	-1.135246000	1.151509000	-1.787579000
H	-2.651243000	0.351379000	-2.303961000
H	-2.714591000	1.897746000	-1.417324000
N	-1.536716000	-0.772076000	1.523655000
N	-2.164100000	0.233317000	-0.257262000
N	1.197531000	0.481566000	-3.055383000
N	2.096851000	2.187377000	-2.129326000
N	2.242992000	1.016411000	2.765937000
N	0.819919000	2.434889000	2.031617000
N	1.768982000	-2.922686000	-0.368037000
N	3.472695000	-1.636903000	-0.509974000
C	-4.692855000	0.242246000	-0.063386000
H	-4.844162000	1.326439000	-0.179378000
H	-4.900418000	-0.222922000	-1.039067000
H	-5.454995000	-0.118220000	0.636033000
C	-3.715957000	-1.299144000	2.703912000
H	-3.582466000	-2.388192000	2.794916000
H	-3.440167000	-0.853520000	3.671558000
H	-4.785414000	-1.115744000	2.554431000
C	5.368130000	-3.226474000	-1.059202000
H	5.731479000	-2.683122000	-1.944479000
H	6.032128000	-2.967562000	-0.220089000
H	5.499645000	-4.295684000	-1.257335000
C	2.733840000	-5.223474000	-0.823523000
H	2.353763000	-5.707809000	0.088853000
H	2.059709000	-5.503445000	-1.647453000
H	3.712479000	-5.665020000	-1.040849000
C	2.965473000	3.530526000	-4.097237000
H	2.459585000	4.475246000	-3.846204000
H	4.009744000	3.619150000	-3.760804000
H	2.982331000	3.452524000	-5.189732000
C	1.588161000	0.876698000	-5.527556000
H	2.042977000	-0.103653000	-5.734987000
H	0.539856000	0.828518000	-5.860565000
H	2.095936000	1.611054000	-6.162085000
C	0.715746000	4.173605000	3.872105000
H	0.961384000	5.055392000	3.260405000
H	-0.377355000	4.156510000	3.998096000
H	1.154846000	4.334680000	4.862564000
C	2.932828000	1.986069000	5.005430000
H	2.708071000	1.102820000	5.622781000
H	4.017350000	1.986608000	4.817970000
H	2.708249000	2.870541000	5.611365000

Sum of electronic and thermal Energies= -2796.288864

Sum of electronic and thermal Enthalpies= -2796.287920

Sum of electronic and thermal Free Energies= -2796.414740
Lowest vibration frequencies (/cm^-1) : 26.6718 27.7626 30.8862

	^{2}**12**		
Fe	0.993777000	0.099356000	0.035122000
C	1.641566000	2.745663000	3.289734000
C	2.692491000	1.904500000	3.550890000
C	2.492490000	-3.959686000	-0.443978000
C	3.601996000	-3.201202000	-0.717399000
C	-3.289555000	-0.166013000	-0.078200000
C	-2.976262000	-0.699630000	1.144014000
C	1.718185000	1.561222000	-3.806989000
C	2.151841000	2.686629000	-3.157429000
C	-0.976610000	-0.137660000	0.100760000
C	1.903798000	-1.746270000	-0.102628000
C	1.685436000	1.152847000	1.604359000
C	1.321342000	1.247937000	-1.539018000
C	-0.139667000	2.859228000	1.553511000
H	-0.022809000	3.942737000	1.423927000
H	-0.307925000	2.378535000	0.585200000
H	-1.010214000	2.671403000	2.197237000
C	3.589446000	-0.177755000	2.543950000
H	3.209934000	-0.914883000	1.834668000
H	4.611141000	0.118617000	2.268187000
H	3.615690000	-0.631130000	3.542913000
C	2.300101000	3.447187000	-0.807599000
H	2.260614000	2.974015000	0.171732000
H	3.326364000	3.788475000	-0.992453000
H	1.633123000	4.320854000	-0.825099000
C	0.742370000	-0.616898000	-3.110216000
H	1.570584000	-1.284730000	-3.384227000
H	0.261752000	-1.009580000	-2.209233000
H	0.018272000	-0.596541000	-3.934329000
C	4.095307000	-0.763989000	-0.796453000
H	5.056654000	-0.874611000	-0.279152000
H	4.282363000	-0.682831000	-1.876141000
H	3.598327000	0.150870000	-0.460191000
C	0.143432000	-3.500075000	0.208455000
H	0.095618000	-4.004881000	1.183690000
H	-0.506773000	-2.626030000	0.212607000
H	-0.207816000	-4.196762000	-0.563115000
C	-0.870448000	-1.051405000	2.425817000
H	0.192862000	-1.127582000	2.170236000
H	-0.985693000	-0.291390000	3.211321000
H	-1.231665000	-2.013991000	2.808759000
C	-2.037676000	0.900014000	-1.928101000
H	-1.026051000	1.278649000	-2.070544000
H	-2.317722000	0.256327000	-2.773603000
H	-2.730121000	1.751141000	-1.895484000
N	-1.590207000	-0.673807000	1.229890000
N	-2.078507000	0.179404000	-0.676474000

N	1.223224000	0.716146000	-2.822310000
N	1.913959000	2.471785000	-1.800937000
N	2.689127000	0.952165000	2.535449000
N	1.055596000	2.277245000	2.121424000
N	1.488148000	-3.062696000	-0.090955000
N	3.223540000	-1.881624000	-0.508036000
C	3.690762000	1.919031000	4.655673000
H	3.546218000	2.800587000	5.289542000
H	3.609911000	1.034817000	5.306718000
H	4.723674000	1.954749000	4.278184000
C	1.144366000	3.936877000	4.032013000
H	1.202454000	4.857103000	3.430621000
H	0.096696000	3.818312000	4.347039000
H	1.738435000	4.102133000	4.937311000
C	4.969181000	-3.601285000	-1.150946000
H	5.248750000	-3.144434000	-2.112183000
H	5.737777000	-3.315152000	-0.416638000
H	5.030046000	-4.687473000	-1.277900000
C	2.297362000	-5.435354000	-0.477888000
H	1.959664000	-5.829946000	0.492081000
H	1.557660000	-5.742999000	-1.232954000
H	3.238198000	-5.939715000	-0.723280000
C	-3.853378000	-1.229641000	2.224272000
H	-4.908590000	-1.111704000	1.955127000
H	-3.682615000	-2.300791000	2.413055000
H	-3.699610000	-0.701205000	3.177142000
C	-4.610367000	0.038475000	-0.734599000
H	-4.843769000	1.103338000	-0.889020000
H	-4.663109000	-0.453917000	-1.717197000
H	-5.412605000	-0.381507000	-0.118343000
C	1.725256000	1.212971000	-5.254685000
H	2.189456000	2.014025000	-5.839849000
H	2.292434000	0.291693000	-5.456252000
H	0.709510000	1.065413000	-5.652791000
C	2.758497000	3.937311000	-3.691160000
H	2.180858000	4.830695000	-3.410069000
H	3.789478000	4.088185000	-3.335611000
H	2.795770000	3.906851000	-4.785443000

Sum of electronic and thermal Energies= -2796.244675
Sum of electronic and thermal Enthalpies= -2796.243731
Sum of electronic and thermal Free Energies= -2796.370759
Lowest vibration frequencies (/cm^-1) : 12.8327 29.7854 31.5008

Structures computed using the def2-TZVP basis set for all atoms.

^{4}1'$_{def2TZVP}$

Fe	-0.002629000	-0.118403000	-0.573150000
C	1.247503000	-0.032524000	2.208124000
C	-1.246942000	-0.033642000	2.208826000
C	0.000450000	-0.059290000	2.832976000
H	0.000732000	-0.066006000	3.919672000

C	0.090354000	-1.668075000	-2.107737000
C	-1.175022000	-1.039569000	-2.239123000
C	1.263215000	-0.884577000	-2.251168000
C	-1.263860000	0.359522000	-2.371008000
H	-2.082337000	-1.632070000	-2.173699000
C	1.175033000	0.517385000	-2.354718000
H	2.239005000	-1.354615000	-2.178030000
C	-0.091436000	1.156806000	-2.345891000
H	-2.239663000	0.835186000	-2.388536000
H	2.082421000	1.113036000	-2.374703000
H	-0.160186000	2.238584000	-2.423545000
N	1.496254000	-0.018489000	0.904926000
N	-1.496824000	-0.020738000	0.905787000
H	0.158977000	-2.747615000	-2.002926000
H	2.116261000	-0.007500000	2.877747000
H	-2.115358000	-0.009358000	2.878874000
C	-2.878510000	0.058920000	0.574064000
C	-3.468160000	1.323186000	0.351870000
C	-3.651939000	-1.118029000	0.471867000
C	-4.816177000	1.382906000	-0.011699000
C	-4.996689000	-1.008085000	0.103483000
C	-5.579108000	0.228438000	-0.146101000
H	-5.272974000	2.357284000	-0.186161000
H	-5.595414000	-1.915170000	0.017158000
H	-6.626984000	0.293099000	-0.436828000
C	2.877846000	0.059066000	0.572348000
C	3.648082000	-1.119839000	0.466545000
C	3.471026000	1.321975000	0.352497000
C	4.992862000	-1.013216000	0.097614000
C	4.818699000	1.378377000	-0.013275000
C	5.578317000	0.222155000	-0.150735000
H	5.588696000	-1.921927000	0.008527000
H	5.277959000	2.351745000	-0.186969000
H	6.625925000	0.284463000	-0.442927000
C	-2.686950000	2.592062000	0.538939000
H	-2.537534000	2.812351000	1.604357000
H	-1.688595000	2.527212000	0.095897000
H	-3.214007000	3.443687000	0.096847000
C	-3.076454000	-2.469056000	0.790369000
H	-2.036604000	-2.562030000	0.465111000
H	-3.081655000	-2.655196000	1.873075000
H	-3.666116000	-3.264387000	0.322403000
C	3.066707000	-2.469822000	0.777970000
H	3.054391000	-2.655354000	1.860642000
H	2.031699000	-2.561151000	0.436985000
H	3.661953000	-3.266165000	0.319033000
C	2.694697000	2.593152000	0.545129000
H	1.691848000	2.530114000	0.112191000
H	2.556834000	2.815402000	1.611730000
H	3.219597000	3.442895000	0.096799000

Sum of electronic and thermal Energies= -2341.873080

Sum of electronic and thermal Enthalpies= -2341.872136
Sum of electronic and thermal Free Energies= -2341.965118
Lowest vibration frequencies (/cm^-1) : 2.6641 41.0434 42.1015

^{2}**1'**$_{\text{def2TZVP}}$

Fe	-0.000985000	-0.110764000	-0.559077000
C	1.224500000	-0.017959000	2.128065000
C	-1.221965000	-0.017410000	2.130411000
C	0.001901000	-0.033994000	2.787666000
H	0.002966000	-0.028646000	3.873335000
C	0.065651000	-1.652903000	-1.980194000
C	-1.179433000	-0.992313000	-2.050259000
C	1.240848000	-0.873030000	-2.062145000
C	-1.245546000	0.416667000	-2.159825000
H	-2.102383000	-1.553910000	-1.942066000
C	1.175286000	0.535815000	-2.170335000
H	2.212942000	-1.344782000	-1.956482000
C	-0.069876000	1.198603000	-2.201551000
H	-2.217588000	0.899433000	-2.128480000
H	2.098363000	1.107848000	-2.152838000
H	-0.123918000	2.283730000	-2.263502000
N	1.417518000	-0.023616000	0.814202000
N	-1.417170000	-0.023538000	0.816927000
H	0.119621000	-2.734173000	-1.869400000
H	2.123401000	0.012206000	2.752498000
H	-2.119729000	0.013266000	2.756432000
C	-2.807907000	0.044729000	0.479973000
C	-3.412336000	1.305563000	0.285175000
C	-3.575678000	-1.136611000	0.407379000
C	-4.768021000	1.355731000	-0.051203000
C	-4.928837000	-1.036376000	0.065971000
C	-5.523775000	0.195522000	-0.174224000
H	-5.236168000	2.327107000	-0.211485000
H	-5.523677000	-1.947419000	-0.003291000
H	-6.577331000	0.252660000	-0.445556000
C	2.807781000	0.048294000	0.475835000
C	3.576702000	-1.132376000	0.399114000
C	3.411164000	1.310178000	0.287032000
C	4.930655000	-1.029937000	0.062556000
C	4.767767000	1.362484000	-0.046410000
C	5.525037000	0.203640000	-0.171229000
H	5.526344000	-1.940246000	-0.008642000
H	5.235622000	2.334840000	-0.201653000
H	6.579420000	0.262876000	-0.438858000
C	-2.643011000	2.580768000	0.476669000
H	-2.541953000	2.821256000	1.543793000
H	-1.627353000	2.507905000	0.078279000
H	-3.154778000	3.422021000	-0.001942000
C	-2.992647000	-2.481446000	0.738588000
H	-1.934612000	-2.549423000	0.473991000
H	-3.060879000	-2.679844000	1.817335000

H	-3.540058000	-3.281773000	0.229264000
C	2.990894000	-2.478652000	0.718151000
H	3.031726000	-2.676106000	1.798390000
H	1.939840000	-2.549792000	0.427485000
H	3.553047000	-3.277424000	0.222849000
C	2.642578000	2.584847000	0.486773000
H	1.622639000	2.512010000	0.099573000
H	2.553854000	2.824864000	1.555157000
H	3.148763000	3.426712000	0.003230000

Sum of electronic and thermal Energies= -2341.886583
Sum of electronic and thermal Enthalpies= -2341.885639
Sum of electronic and thermal Free Energies= -2341.971362
Lowest vibration frequencies (/cm^-1) : 16.7020 46.4039 50.6926

$^{4}2'_{def2TZVP}$

Fe	0.034712000	-0.850737000	-0.446702000
C	-1.269853000	-3.559026000	-0.067966000
C	1.176179000	-3.671977000	-0.509581000
C	-0.059686000	-4.241758000	-0.199143000
H	-0.091643000	-5.321309000	-0.082256000
N	-1.488722000	-2.255003000	-0.172835000
N	1.413450000	-2.385756000	-0.682440000
H	-2.147184000	-4.184918000	0.135429000
H	2.022205000	-4.359581000	-0.629309000
C	2.735421000	-2.003895000	-1.050802000
C	3.075648000	-1.913633000	-2.421310000
C	3.689945000	-1.698446000	-0.054107000
C	4.342273000	-1.436689000	-2.766402000
C	4.944622000	-1.227162000	-0.453132000
C	5.268755000	-1.077503000	-1.794825000
H	4.603524000	-1.353095000	-3.821257000
H	5.680670000	-0.979782000	0.311990000
H	6.247515000	-0.696831000	-2.083915000
C	-2.857630000	-1.876943000	-0.015657000
C	-3.378280000	-1.642149000	1.275051000
C	-3.677168000	-1.750355000	-1.157846000
C	-4.715519000	-1.252285000	1.395134000
C	-5.007634000	-1.358869000	-0.985045000
C	-5.527913000	-1.104925000	0.278052000
H	-5.121102000	-1.063308000	2.388904000
H	-5.644235000	-1.256145000	-1.863675000
H	-6.566240000	-0.796046000	0.391541000
C	2.146540000	-2.378261000	-3.507125000
H	1.094607000	-2.297057000	-3.227494000
H	2.308531000	-1.811997000	-4.430031000
H	2.329924000	-3.436790000	-3.740019000
C	3.435086000	-1.929086000	1.409488000
H	2.376850000	-2.054018000	1.641123000
H	3.947748000	-2.842487000	1.742028000
H	3.829082000	-1.104272000	2.013306000
C	-2.541246000	-1.818873000	2.508960000

H	-2.331044000	-2.877672000	2.708548000
H	-1.570399000	-1.321531000	2.420000000
H	-3.055473000	-1.413866000	3.385826000
C	-3.159359000	-2.048525000	-2.534836000
H	-2.248260000	-1.484404000	-2.759241000
H	-2.904334000	-3.109460000	-2.651296000
H	-3.909615000	-1.800977000	-3.291858000
C	0.692618000	0.163867000	0.988655000
C	0.225142000	0.150620000	-2.024218000
C	-1.443674000	0.614120000	-0.226436000
O	1.058211000	0.829728000	1.855567000
O	0.329090000	0.809582000	-2.963868000
O	-1.781094000	1.715312000	-0.184127000

Sum of electronic and thermal Energies= -2449.678708
Sum of electronic and thermal Enthalpies= -2449.677764
Sum of electronic and thermal Free Energies= -2449.775437
Lowest vibration frequencies (/cm^-1) : 12.1687 27.3835 42.4242

^{2}**2'**$_{\text{def2TZVP}}$

Fe	-0.131380000	-0.874956000	-0.963401000
C	-1.354100000	-3.544557000	-0.589814000
C	1.063930000	-3.581893000	-0.998956000
C	-0.175545000	-4.210698000	-0.915537000
H	-0.202399000	-5.294201000	-0.975299000
N	-1.519473000	-2.237368000	-0.478403000
N	1.296548000	-2.280825000	-0.952745000
H	-2.229137000	-4.163555000	-0.365139000
H	1.944953000	-4.228161000	-1.073202000
C	2.690995000	-1.939265000	-0.928230000
C	3.426053000	-1.848054000	-2.128312000
C	3.316116000	-1.731181000	0.321046000
C	4.782961000	-1.514215000	-2.050449000
C	4.671947000	-1.397341000	0.342413000
C	5.405143000	-1.281855000	-0.832245000
H	5.357178000	-1.441347000	-2.973888000
H	5.158387000	-1.235203000	1.303869000
H	6.462139000	-1.021482000	-0.796551000
C	-2.817114000	-1.851801000	-0.000095000
C	-2.988535000	-1.631203000	1.384202000
C	-3.902557000	-1.729436000	-0.891935000
C	-4.249263000	-1.252041000	1.849897000
C	-5.146527000	-1.353461000	-0.372276000
C	-5.324472000	-1.107666000	0.981756000
H	-4.385450000	-1.076997000	2.916718000
H	-5.990686000	-1.256407000	-1.054701000
H	-6.301610000	-0.812963000	1.362106000
C	2.815622000	-2.076779000	-3.482361000
H	1.996904000	-2.799395000	-3.465354000
H	2.414114000	-1.143232000	-3.896703000
H	3.574080000	-2.438909000	-4.184123000
C	2.567385000	-1.870725000	1.614534000

H	1.737602000	-1.157925000	1.682049000
H	2.132247000	-2.870066000	1.730928000
H	3.233246000	-1.692367000	2.464049000
C	-1.859794000	-1.811950000	2.356544000
H	-1.534807000	-2.858457000	2.411089000
H	-0.979743000	-1.226707000	2.070112000
H	-2.163545000	-1.503381000	3.361244000
C	-3.780783000	-1.966086000	-2.370859000
H	-3.514879000	-1.040476000	-2.897097000
H	-3.022192000	-2.709602000	-2.624530000
H	-4.738168000	-2.303888000	-2.781025000
C	1.067998000	0.405938000	-0.892345000
C	-0.428514000	-0.638977000	-2.718003000
C	-1.197456000	0.441260000	-0.497487000
O	1.770072000	1.325817000	-0.883012000
O	-0.611008000	-0.312755000	-3.812245000
O	-1.825441000	1.382622000	-0.255382000

Sum of electronic and thermal Energies= -2449.735443
Sum of electronic and thermal Enthalpies= -2449.734499
Sum of electronic and thermal Free Energies= -2449.825967
Lowest vibration frequencies (/cm^-1) : 22.7327 32.1036 41.5226

$^{4}\mathbf{4}_{\mathbf{Me,def2TZVP}}$

C	3.811816000	-1.736686000	0.366053000
C	2.753492000	-0.846856000	0.573463000
C	1.685183000	-0.699160000	-0.333952000
C	1.752615000	-1.529538000	-1.471726000
C	2.800686000	-2.422559000	-1.700845000
C	3.843143000	-2.531065000	-0.779088000
H	4.615945000	-1.813716000	1.103208000
H	2.769942000	-0.247903000	1.489768000
H	0.947229000	-1.488750000	-2.210792000
H	2.804385000	-3.043893000	-2.600468000
H	4.664202000	-3.230063000	-0.947951000
Fe	0.113883000	0.601846000	-0.086318000
C	0.765711000	2.360065000	-0.888737000
C	-0.589042000	2.249028000	-1.372217000
C	0.898369000	2.418246000	0.528035000
C	-1.669591000	2.750963000	-0.566731000
C	-0.256564000	2.420466000	1.357995000
H	1.890885000	2.395189000	0.977375000
C	-1.513479000	2.811883000	0.796521000
H	-2.632205000	2.974290000	-1.027754000
H	-0.127491000	2.385063000	2.438581000
H	-2.347649000	3.070331000	1.448447000
H	-0.734103000	2.148270000	-2.447822000
C	-1.521187000	-0.576175000	0.116983000
C	-2.698029000	-0.572368000	-0.660835000
C	-1.482174000	-1.575809000	1.116599000
C	-3.746669000	-1.476512000	-0.465431000
H	-2.809517000	0.167676000	-1.455279000

C	-2.523953000	-2.478190000	1.336944000
H	-0.596742000	-1.664012000	1.751148000
C	-3.670786000	-2.436174000	0.542371000
H	-4.631529000	-1.430910000	-1.106711000
H	-2.439895000	-3.223804000	2.132285000
H	-4.487372000	-3.142509000	0.703418000
C	1.929839000	2.507998000	-1.820272000
H	2.065261000	3.561797000	-2.116100000
H	2.862117000	2.164197000	-1.358386000
H	1.781605000	1.925627000	-2.737938000

Sum of electronic and thermal Energies= -1998.470721
Sum of electronic and thermal Enthalpies= -1998.469777
Sum of electronic and thermal Free Energies= -1998.543141
Lowest vibration frequencies (/cm^-1) : 23.1862 31.4424 36.9920

$^{2}\mathbf{4}_{\mathbf{Me,def2TZVP}}$

C	3.166566000	-1.834290000	0.733370000
C	2.142305000	-0.895208000	0.869457000
C	1.325870000	-0.484596000	-0.208592000
C	1.611772000	-1.120257000	-1.437849000
C	2.636023000	-2.055376000	-1.590818000
C	3.429894000	-2.422983000	-0.503712000
H	3.766171000	-2.110254000	1.605461000
H	1.976548000	-0.465605000	1.860151000
H	1.007670000	-0.883902000	-2.316174000
H	2.811119000	-2.509928000	-2.570023000
H	4.228984000	-3.157614000	-0.616253000
Fe	-0.046745000	0.903933000	-0.021405000
C	0.729225000	2.497266000	-1.130669000
C	-0.690372000	2.457676000	-1.223200000
C	1.319692000	2.473462000	0.163411000
C	-1.485841000	2.411462000	-0.050223000
C	0.532708000	2.346350000	1.337501000
H	2.403069000	2.381629000	0.242119000
C	-0.880045000	2.325809000	1.228986000
H	-2.561872000	2.268758000	-0.142393000
H	1.016192000	2.245413000	2.309909000
H	-1.498425000	2.165255000	2.112110000
H	-1.170704000	2.443345000	-2.202760000
C	-1.376905000	-0.526278000	0.108064000
C	-2.136167000	-0.962102000	-1.000923000
C	-1.705554000	-1.152673000	1.331210000
C	-3.148515000	-1.918102000	-0.899953000
H	-1.936885000	-0.537311000	-1.987518000
C	-2.717720000	-2.106375000	1.447927000
H	-1.150169000	-0.888056000	2.233848000
C	-3.454982000	-2.499954000	0.330317000
H	-3.705115000	-2.212346000	-1.794276000
H	-2.929525000	-2.552978000	2.423525000
H	-4.245674000	-3.247254000	0.415104000
C	1.584490000	2.574205000	-2.362488000

H	1.803154000	3.621228000	-2.628098000
H	2.541485000	2.061012000	-2.217611000
H	1.086608000	2.112922000	-3.223692000

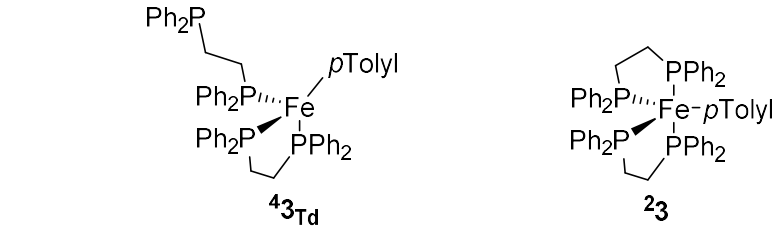
Sum of electronic and thermal Energies= -1998.512741
Sum of electronic and thermal Enthalpies= -1998.511797
Sum of electronic and thermal Free Energies= -1998.580370
Lowest vibration frequencies (/cm^-1) : 30.8272 35.2477 40.3843

Comparison between the doublet-quartet gaps computed using def2-TZVP basis set on Fe and 6-31G on other atoms (level A) and using def2-TZVP basis set on all atoms (level B):*

	Level A	Level B
1'	G_Q-G_D = 5.7 E_Q-E_D = 8.8	G_Q-G_D = 3.9 E_Q-E_D = 8.4
2'	G_Q-G_D = 32.5 E_Q-E_D = 35.6	G_Q-G_D = 31.7 E_Q-E_D = 35.6
4_{Me}	G_Q-G_D = 22.8 E_Q-E_D = 25.6	G_Q-G_D = 23.6 E_Q-E_D = 26.4

Table S1. Computed doublet-quartet gaps (in kcal.mol^{-1}) for complexes **1'**, **2'** and **4_{Me}**.

*Optimization of ^{2}**3** and ^{4}**3_{Td}** at the OPBE level (without dispersion) :*

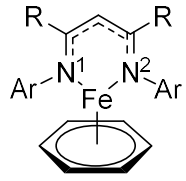
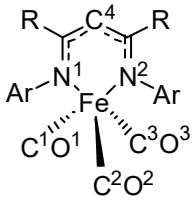
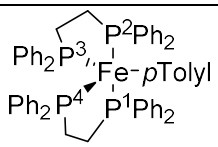
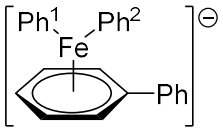
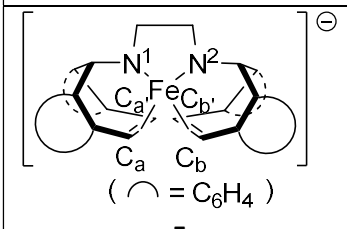
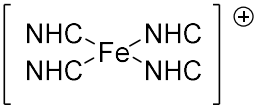


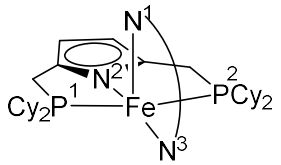
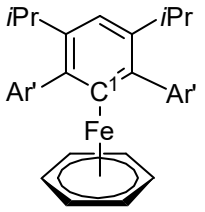
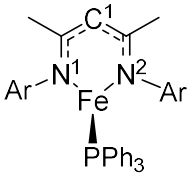
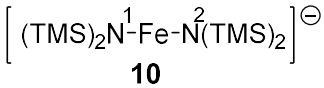
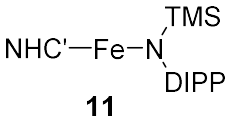
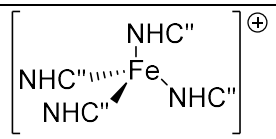
^{4}**3_{Td}** ^{2}**3**

G (/kcal.mol^{-1})	0.0	12.5
E (/kcal.mol^{-1})	0.0	7.6

Scheme S1. Comparison between the thermodynamic features of ^{4}**3_{Td}** and ^{2}**3**.

3) Comparison between metric parameters of experimental and computed structures

Complex	Selected metric parameters[a]	Experimental value	Computed Value[b]	% Error[b]
 **1**	N^1—Fe	1.97	2.02	3
	N^2—Fe	1.98	2.03	3
	N^1—Fe—N^2	92.2	92.9	1
	Average Fe—C_{arene}	2.14	2.11	1
 **2**	N^1—Fe	1.98	2.02	2
	N^2—Fe	1.98	2.02	2
	C^1—Fe	1.80	1.76	2
	C^2—Fe	1.87	1.79	4
	C^3—Fe	1.80	1.76	2
	N^1—Fe—N^2	91.0	93.1	2
	N^1—Fe—C^3	163.2	163.1	0
	N^2—Fe—C^1	163.2	162.6	0
	O^1—C^1—Fe	174.9	172.9	1
	O^2—C^2—Fe	179.5	171.7	4
	O^2—C^3—Fe	174.9	172.9	1
	C^4—Fe—C^2	90.9	94.7	4
 **3**	P^1—Fe	2.22	2.26	2
	P^2—Fe	2.24	2.25	1
	P^3—Fe	2.23	2.31	4
	P^4—Fe	2.25	2.24	1
	C—Fe	2.05	2.02	1
	P^3—Fe—P^4	104.7	97.6	7
	P^3—Fe—C	133.5	146.4	10
	P^4—Fe—C	121.8	115.8	5
	P^1—Fe—P^2	178.3	173.2	3
 **4_{Ph}**	Ph^1—Fe	1.98	1.97	1
	Ph^2—Fe	1.97	1.96	1
	Average Fe—C_{arene}	2.11	2.08	1
	Ph^1—Fe—Ph^2	93.1	88.6	4
 **5**	N^1—Fe	1.90	1.85	3
	N^2—Fe	1.95	1.85	5
	C_a $C_{a'}$—Fe	1.92	1.87	3
	C_b $C_{b'}$—Fe	1.93	1.87	3
	N^1—Fe—N^2	79.2	84.9	7
 **6**	C^1—Fe	2.00	2.05	3
	C^2—Fe	2.00	2.05	3
	C^3—Fe	2.00	2.05	3
	C^4—Fe	1.98	2.05	4
	C^2—Fe—C^1	89.6	90.0	1
	C^3—Fe—C^2	89.8	90.0	1
	C^4—Fe—C^1	89.5	89.7	1
	C^4—Fe—C^3	91.1	90.2	1

 **7** N N = 2,2'-bipyridine	N^1—Fe	1.96	1.93	2
	N^2—Fe	1.97	1.95	1
	N^3—Fe	1.91	1.88	2
	P^1—Fe	2.28	2.31	1
	P^2—Fe	2.32	2.31	1
	N^2—Fe—N^3	174.4	179.6	3
	N^2—Fe—N^1	92.8	98.1	6
	N^1—Fe—N^3	81.6	82.2	1
	P^1—Fe—N^1	105.0	101.6	3
	P^2—Fe—N^1	105.1	101.3	4
	P^1—Fe—N^3	100.4	98.4	2
	P^2—Fe—N^3	102.4	98.9	3
 **8**	C^1—Fe	2.03	2.06	1
	Average Fe—C_{arene}	2.16	2.15	1
 **9**	Fe—P	2.23	2.29	3
	Fe—N^1	1.95	2.00	3
	Fe—N^2	1.96	2.00	2
	N^1—Fe—N^2	98.1	100.7	3
	N^1—Fe—P	127.3	126.4	1
	N^2—Fe—P	125.3	126.3	1
	C^1—Fe—P		153.7	
 **10**	Fe—N^1	1.92	1.91	1
	Fe—N^2	1.92	1.92	0
	N^1—Fe—N^2	180	179.3	4
 **11**	Fe—$C_{NHC'}$	2.01	1.96	2
	Fe—N	1.89	1.91	1
	$C_{NHC'}$—Fe—N	176.9	173.4	2
	Fe—N—C_{DIPP}	115.8	123.2	6
	Fe—N—C_{TMS}	118.1	114.8	3
 **12**	C^1—Fe	2.06	2.07	1
	C^2—Fe	2.05	2.07	1
	C^3—Fe	2.04	2.07	1
	C^4—Fe	2.04	2.07	1
	C^2—Fe—C^1	112.4	116.0	3
	C^3—Fe—C^1	117.1	115.3	2
	C^3—Fe—C^2	98.9	97.8	1
	C^4—Fe—C^1	101.4	97.6	4
	C^4—Fe—C^2	116.0	115.6	1
	C^4—Fe—C^3	111.8	115.7	3

[a] bonds in Å, angles in degrees; [b] for non-truncated computed complexes.

Table S2. Comparison between the computed metric parameters of benchmarked complexes and experimental data.

4) Analysis of α/β population for complexes ^{2}**4**$_{Me}$ and ^{2}**1'** upon arene decoordination

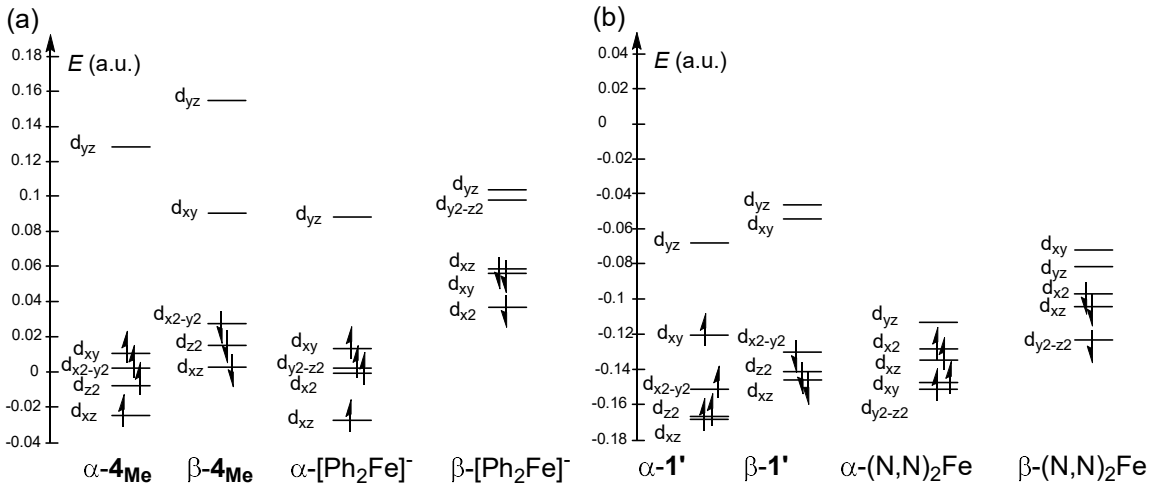


Figure S1. Evolution of the alpha and beta d-block MOs span of complexes ^{2}**4**$_{Me}$ (*a*) and ^{2}**1'** (*b*) upon decoordination of the η^6-arene ligand.

5) Computation of Mössbauer isomer shifts

Mössbauer parameters can be evaluated easily using DFT techniques, which allow the computation of the electronic density at the ^{57}Fe nucleus, noted ρ_0 (unit: e.a_0^{-3}, where a_0 is Bohr radius). A reliable estimation of the isomer shift (δ) can be obtained with a linear extrapolation from ρ_0.[4] All calculations were performed with ORCA 3.0.3 software,[5] using the OPBE functional in gas phase, associated with the TZVP basis set[6a] for all atoms except Fe which was treated with the CP(PPP) enlarged basis set.[6b,c] This choice has been motivated since it allows a good compromise between accuracy and computational time. It has indeed been demonstrated that the use of CP(PPP) basis set on iron allowed more accurate linear fit between ρ_0 and δ for a very modest additional computational cost.[4]

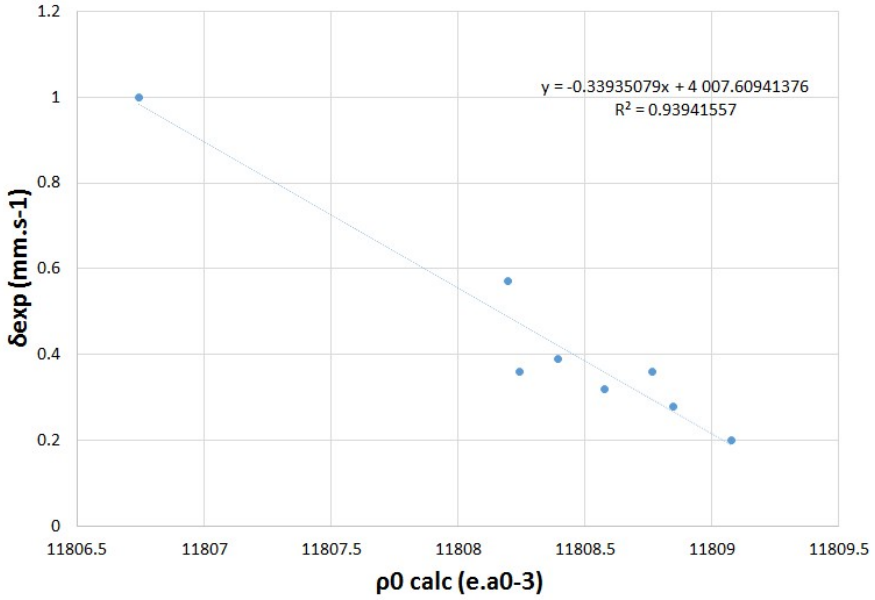
Computed isomer shifts:

Complex	ρ_0 (e.a_0^{-3})	δ_{exp} (mm.s^{-1}) [ref]
3	11808.57503	0.32 [7a]
4_{Me}	11808.84611	0.28 [7b]
5	11809.07564	0.20 [7c]
6	11808.24062	0.36 [7d]
10	11808.76521	0.36 [7e]
11	11808.39345	0.39 [7f]
12	11808.19616	0.57 [7d]
$[FeCl_4]^{2-}$ (S = 2, T_d)	11806.74303	1.00 [7g]

Table S3. Computed electronic densities and experimental isomer shifts of selected complexes.

The calibration curve $\rho_{0,calc} = f(\delta_{exp})$ is given thereafter.

The values of computed isomer shifts (δ_{calc}) reported in the article (Table 1) have been calculated using the calibration curve equation:



$\delta_{calc} = -0.3393\rho_0 + 4007.6094$ (mm.s^{-1})

Figure S2. Calibration curve $\rho_{0,calc} = f(\delta_{exp})$.

References

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