Supplementary Materials: Hexakis (1-propargyltetrazole) Iron(II) X_2 [X = BF_4, ClO_4]—Spin Switchable Complexes with Functionalization Potential and the Myth of the Explosive SCO Compound

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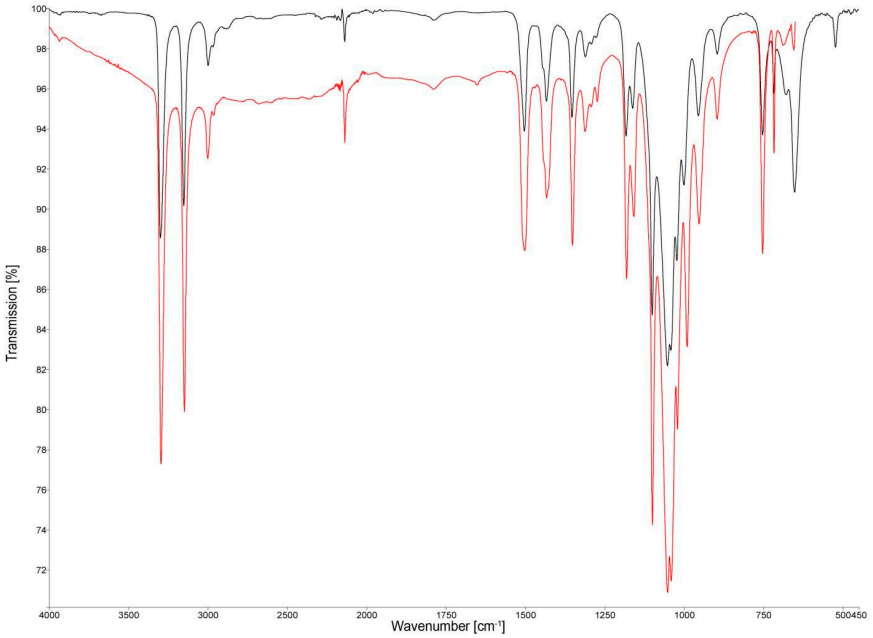

Figure S1. Comparison of the mid-infrared spectra for $[Fe(prgTz)_6](BF_4)_2$ (red) and $[Ni(prgTz)_6](BF_4)_2$ (black).

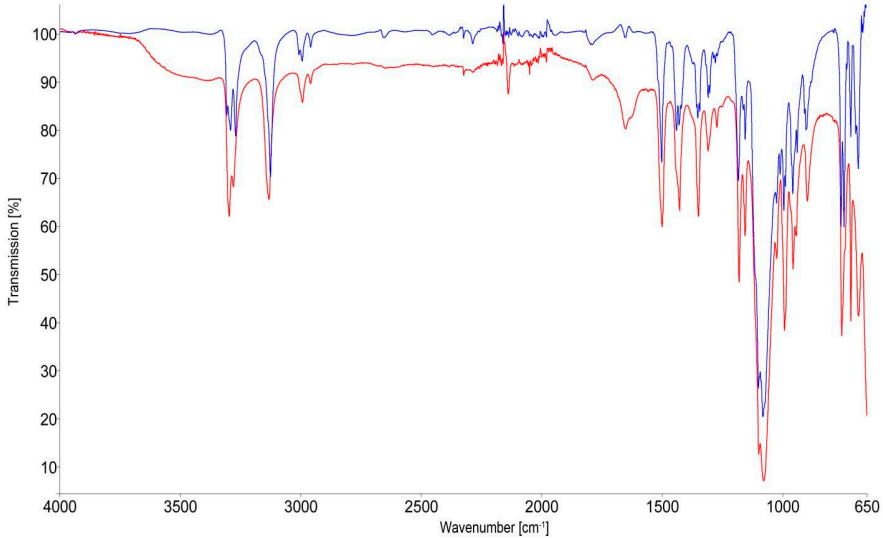

Figure S2. Mid-infrared spectrum of $[Fe(prgTz)_6](ClO_4)_2$, high-spin (red) and low-spin (blue).

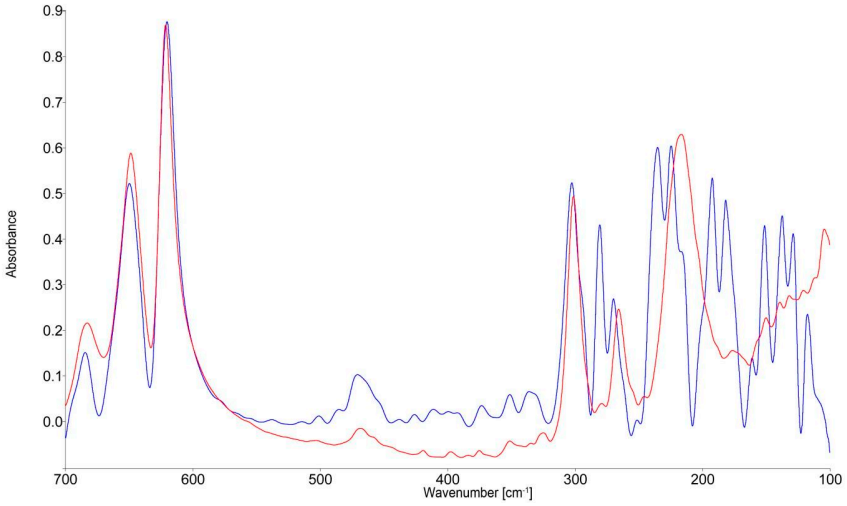

Figure S3. Far-infrared spectrum of $[Fe(prgTz)_6](ClO_4)_2$, high-spin (red) and low-spin (blue).

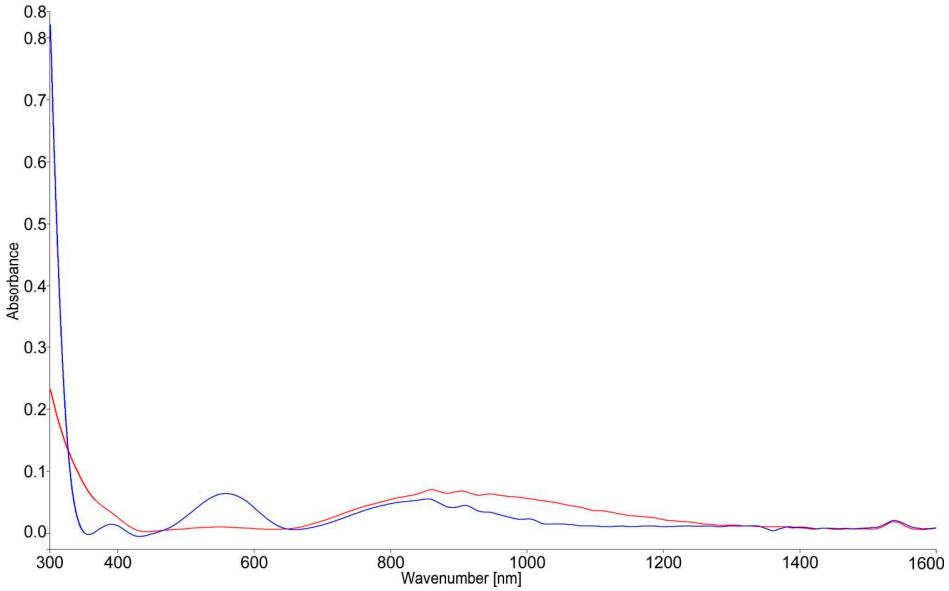

Figure S4. Visible/near-infrared spectrum of $[Fe(prgTz)_6](ClO_4)_2$, high-spin (red) and low-spin (blue).

Table S1. Coordinates of the calculated low-spin structure for the $[Fe(prgTz)_6]^{2+}$ cation.

Atom Name	*x*	*y*	*z*
Fe	0.00000000	0.00000000	0.00000000
N	–0.74545400	–1.86613000	0.09366400
N	0.09049700	–2.97500700	0.23252200
N	–0.62821300	–4.07398000	0.21624900
N	–1.93932000	–3.67900400	0.06294000
C	–1.99418200	–2.33580600	–0.00960700
N	1.00906700	–0.29148800	1.71605400
N	1.17625400	0.73667100	2.64461400
N	1.91150900	0.31125300	3.64616400
N	2.22737700	–1.00053100	3.36691600
C	1.67162900	–1.35205800	2.19224400
N	–1.58062300	0.70805000	1.02304600
N	–2.88840900	0.45029600	0.61009000
N	–3.73203800	1.06001400	1.41074900
N	–2.96931600	1.72095800	2.34890500

C	–1.66522500	1.49720900	2.10030000
H	–2.88260300	–1.74529200	–0.11767400
H	–0.83975500	1.87358800	2.67189300
N	0.74545400	1.86613000	–0.09366400
N	–0.09049700	2.97500700	–0.23252200
N	0.62821300	4.07398000	–0.21624900
N	1.93932000	3.67900400	–0.06294000
C	1.99418200	2.33580600	0.00960700
N	–1.00906700	0.29148800	–1.71605400
N	–1.17625400	–0.73667100	–2.64461400
N	–1.91150900	–0.31125300	–3.64616400
N	–2.22737700	1.00053100	–3.36691600
C	–1.67162900	1.35205800	–2.19224400
N	1.58062300	–0.70805000	–1.02304600
N	2.88840900	–0.45029600	–0.61009000
N	3.73203800	–1.06001400	–1.41074900
N	2.96931600	–1.72095800	–2.34890500
C	1.66522500	–1.49720900	–2.10030000
H	2.88260300	1.74529200	0.11767400
H	0.83975500	–1.87358800	–2.67189300
H	1.73801200	–2.31546500	1.72643800
H	–1.73801200	2.31546500	–1.72643800
C	–3.07226000	1.77353000	–4.31408100
H	–2.61252500	1.67889100	–5.29841600
H	–4.04656800	1.28409900	–4.35235500
C	–3.01443900	–4.70233000	–0.01048200
H	–2.85508000	–5.27629600	–0.92464400
H	–2.86750100	–5.37474400	0.83523500
C	3.63389000	–2.53077200	–3.40291600
H	4.41314200	–1.90346300	–3.83668400
H	4.12044600	–3.37292500	–2.90831000
C	3.07226000	–1.77353000	4.31408100
H	4.04656800	–1.28409900	4.35235500
H	2.61252500	–1.67889100	5.29841600
C	–3.63389000	2.53077200	3.40291600
H	–4.12044600	3.37292500	2.90831000
H	–4.41314200	1.90346300	3.83668400
C	3.01443900	4.70233000	0.01048200
H	2.86750100	5.37474400	–0.83523500
H	2.85508000	5.27629600	0.92464400
C	–4.33888100	–4.10187800	0.01193200
C	2.69222800	–2.98476100	–4.41406400
C	4.33888100	4.10187800	–0.01193200
C	–3.19642400	3.16753400	–3.91842400
C	3.19642400	–3.16753400	3.91842400
C	–2.69222800	2.98476100	4.41406400
C	–5.46568800	–3.67838100	0.02824200
C	1.97390900	–3.39482300	–5.28880400
C	–3.34401400	4.33340000	–3.65708500
C	3.34401400	–4.33340000	3.65708500
C	5.46568800	3.67838100	–0.02824200
C	–1.97390900	3.39482300	5.28880400

H	1.34803300	–3.75994500	–6.06745200
H	6.46488000	3.31411100	–0.04407100
H	3.47861100	–5.36506800	3.43598200
H	–1.34803300	3.75994500	6.06745200
H	–6.46488000	–3.31411100	0.04407100
H	–3.47861100	5.36506800	–3.43598200

Table S2. Coordinates of the calculated high-spin structure for the $[Fe(prgTz)_6]^{2+}$ cation.

Atom Name	*x*	*y*	*z*
Fe	0.00000000	0.00000000	0.00000000
N	–1.29489000	–1.77710500	0.07592200
N	–0.69847300	–3.03706500	0.11554700
N	–1.62842900	–3.96523700	0.09442600
N	–2.83871800	–3.30230700	0.04248100
C	–2.61617300	–1.97353800	0.03262900
N	1.15188900	–0.76777400	1.70741400
N	1.56247800	0.10258700	2.71795100
N	2.25311500	–0.55925000	3.61837400
N	2.29180700	–1.87255400	3.18963300
C	1.61672300	–1.97939800	2.02916300
N	–1.37959500	0.99883500	1.38834400
N	–2.74241700	1.06075800	1.09757800
N	–3.36141000	1.74382700	2.03370900
N	–2.39195300	2.13051800	2.93874200
C	–1.19470400	1.66571500	2.53172700
H	–3.36938600	–1.20972900	0.01299900
H	–0.25958800	1.79145500	3.04312700
N	1.29489000	1.77710500	–0.07592200
N	0.69847300	3.03706500	–0.11554700
N	1.62842900	3.96523700	–0.09442600
N	2.83871800	3.30230700	–0.04248100
C	2.61617300	1.97353800	–0.03262900
N	–1.15188900	0.76777400	–1.70741400
N	–1.56247800	–0.10258700	–2.71795100
N	–2.25311500	0.55925000	–3.61837400
N	–2.29180700	1.87255400	–3.18963300
C	–1.61672300	1.97939800	–2.02916300
N	1.37959500	–0.99883500	–1.38834400
N	2.74241700	–1.06075800	–1.09757800
N	3.36141000	–1.74382700	–2.03370900
N	2.39195300	–2.13051800	–2.93874200
C	1.19470400	–1.66571500	–2.53172700
H	3.36938600	1.20972900	–0.01299900
H	0.25958800	–1.79145500	–3.04312700
H	1.46095200	–2.88269800	1.47178400
H	–1.46095200	2.88269800	–1.47178400
C	–3.01679000	2.88815300	–3.99528300
H	–2.65212700	2.79908700	–5.01904100
H	–4.07251000	2.61289200	–3.99189300
C	–4.10341100	–4.08043000	–0.00102000
H	–4.11846100	–4.62511300	–0.94628900
H	–4.05110600	–4.81269500	0.80513900

C	2.77328100	–2.94026400	–4.12432900
H	3.60519600	–2.42471900	–4.60506900
H	3.14204600	–3.89952900	–3.75799600
C	3.01679000	–2.88815300	3.99528300
H	4.07251000	–2.61289200	3.99189300
H	2.65212700	–2.79908700	5.01904100
C	–2.77328100	2.94026400	4.12432900
H	–3.14204600	3.89952900	3.75799600
H	–3.60519600	2.42471900	4.60506900
C	4.10341100	4.08043000	0.00102000
H	4.05110600	4.81269500	–0.80513900
H	4.11846100	4.62511300	0.94628900
C	–5.27210500	–3.22492900	0.13349700
C	1.65825900	–3.11874600	–5.04118200
C	5.27210500	3.22492900	–0.13349700
C	–2.82074300	4.23327500	–3.47754400
C	2.82074300	–4.23327500	3.47754400
C	–1.65825900	3.11874600	5.04118200
C	–6.28294300	–2.58015700	0.24239600
C	0.78267700	–3.30474100	–5.84624300
C	–2.70155900	5.37274300	–3.10772200
C	2.70155900	–5.37274300	3.10772200
C	6.28294300	2.58015700	–0.24239600
C	–0.78267700	3.30474100	5.84624300
H	0.01612500	–3.47297800	–6.56408400
H	7.18164400	2.01976200	–0.34008000
H	2.60065700	–6.38268300	2.78988600
H	–0.01612500	3.47297800	6.56408400
H	–7.18164400	–2.01976200	0.34008000
H	–2.60065700	6.38268300	–2.78988600