Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary information of

Spin crossover complexes $[Fe(NH_2trz)_3](X)_2.nH_2O$ investigated by means of Raman scattering and DFT calculations.

Yeny A. Tobon[1,3], Lara Kabalan[2], Sébastien Bonhommeau[1], Nathalie Daro[2], Arnaud Grosjean[2], Philippe Guionneau[2], Samir Matar[2], Jean-François Létard[2], François Guillaume[1]

[1]*Université Bordeaux 1, CNRS UMR 5255, ISM, 33405 Talence Cedex, France*

[2]*CNRS UPR 9048, Université Bordeaux 1, ICMCB, 33600 Pessac, France*

[3]*Université de Lille 1, CNRS UMR 8516, LASIR, Bât. C5, 59655 Villeneuve d'Ascq Cedex, France*

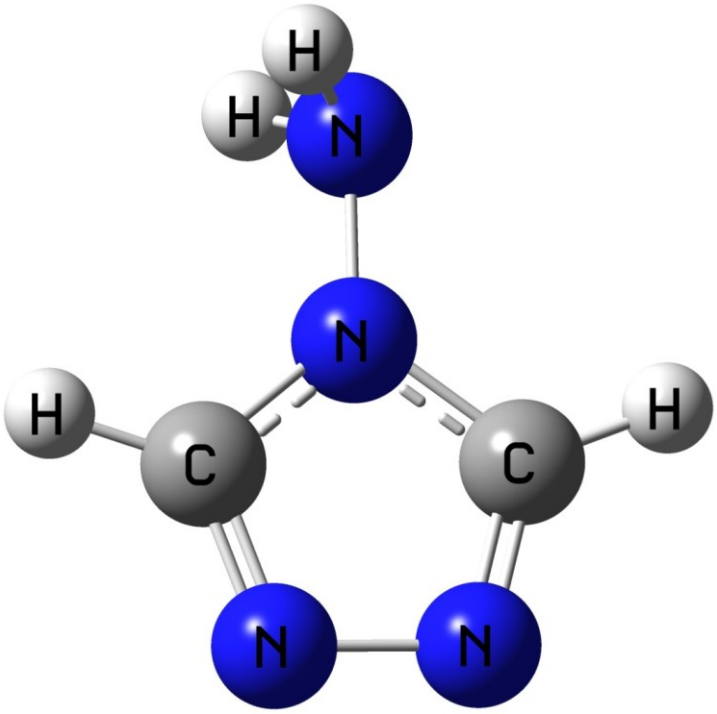

Figure S1.B3LYP/6-31+G* molecular model for 4-NH_2-1,2,4-triazole (NH_2trz).

Table S1. Wavenumbers (cm^{-1}) and assignments of the Raman bands of the NH_2trz molecule calculated with the B3LYP/6-31+G* method. The potential energy distribution (PED) was calculated using the freeware GAR2PED (Martin, J.M.L, Van Alsenoy, C., GAR2PED, *A Program to obtain a Potential Energy Distribution from a Gaussian archive record*, University of Antwerp, Belgium (2007)).

Mode	B3LYP/6-31+G*	Assignment (PED)[a]
1.	205.96	γNH_2 (93%)
2.	270.46	τCN-NH_2 (87%)
3.	387.22	δC-N-NH_2 (84%)
4.	614.33	γrg (86%)
5.	685.01	νN-NH_2 (45%), δrg (30%)
6.	691.57	τrg (95%)
7.	801.36	γCH (82%)
8.	840.19	γCH (75%)
9.	882.46	ωNH_2 (77%)
10.	937.59	δrg (82%)
11.	1005.29	νN-N (89%)

12.	1073.05	δrg (39%), νC-NNH_2 (37%), δH-C-N (16%)
13.	1213.04	δH-C-N (33%), δrg (25%), νN–NH_2 (16%), νN–N (11%)
14.	1217.74	δH-C-N (84%)
15.	1319.73	ρNH_2 (98%)
16.	1335.25	νC-NNH_2 (43%), νC-N (26%)
17.	1410.22	νC-N (50%), νC-NNH_2 (43%)
18.	1502.69	νC-N (78%)
19.	1542.07	νC-N (31%), δH-C-N (27%), νC-NNH_2 (24%)
20.	1687.90	δNH_2 (90%)
21.	3271.47	νC-H (98%)
22.	3290.73	νC-H (98%)
23.	3495.87	νN-H (100%)
24.	3596.21	νN-H (100%)

[a] Meaning of symbols: ν, stretching; δ, deformation or in-plane bending; γ, out-of-plane bending; ω, wagging; τ, torsion; ρ, rocking; rg, ring

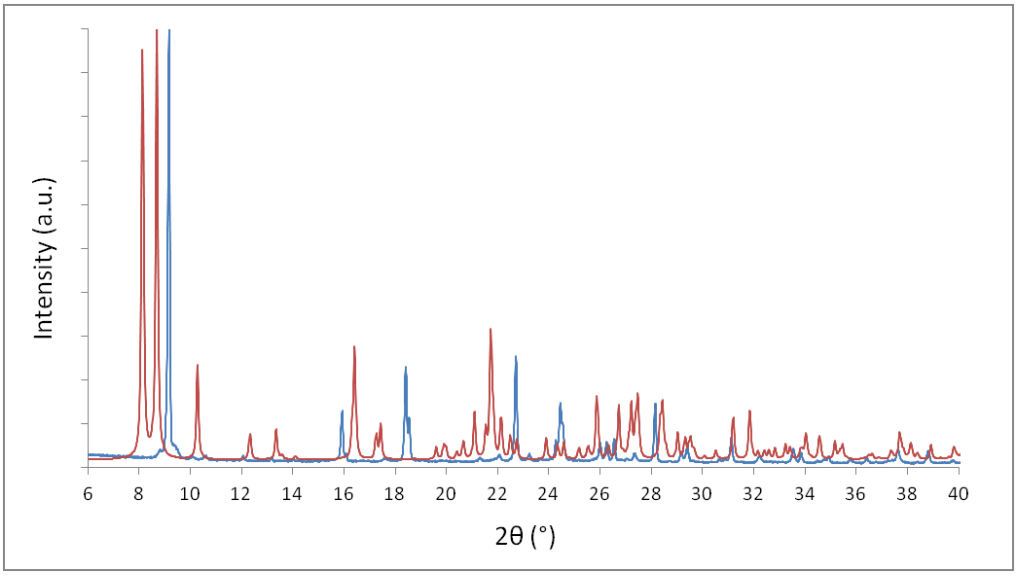

Figure S2: comparison of the powder X-ray diffraction patterns of [Fe(NH_2-trz)$_3$](NO_3)$_2$.2H_2O (red line, derived from the single-crystal pattern) and [Fe(NH_2-trz)$_3$](NO_3)$_2$.H_2O (blue line, experimental pattern).

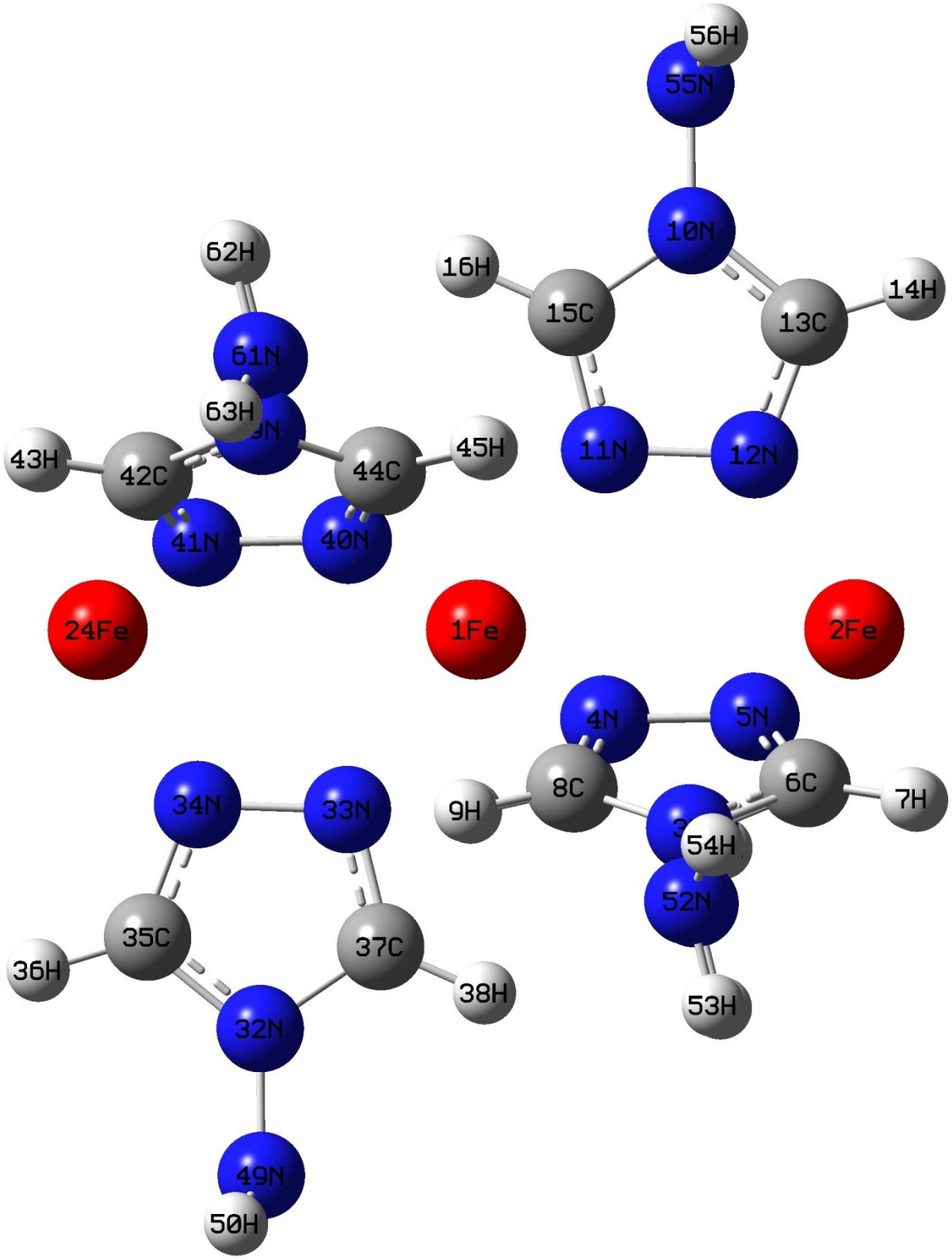

Figure S3. B3LYP/LANL2DZ/6-31+G* molecular model for the polymeric ionic Fe(NH_2-trz)$_3^{2+}$ complex, in the LS state, containing three Fe atoms and six NH_2-trz ligands

Table S2. Cartesian coordinates of the optimized structure for the polymeric ionic Fe(NH_2-trz)$_3^{2+}$ complex, in the LS state, containing three Fe atoms and six NH_2-trz ligands at the B3LYP/LanL2DZ/6-31+G* level of approximation

Atom	X	Y	Z
Fe	0.000001	-0.000012	0.000054
Fe	-3.588869	0.00207	-0.000366
N	-2.051725	-1.809853	-3.323079
N	-1.222884	-0.816021	-1.498201
N	-2.643868	-0.791524	-1.456096
C	-3.118958	-1.392938	-2.56065
H	-4.1573	-1.542152	-2.836915
C	-0.908334	-1.439227	-2.640602
H	0.07666	-1.650542	-3.025964
N	-2.0492	3.784452	0.093863
N	-1.221375	1.706764	0.042542
N	-2.642327	1.658747	0.041442
C	-3.116849	2.916266	0.072572
H	-4.155041	3.230683	0.080608
C	-0.906164	3.007561	0.074371
H	0.079036	3.446431	0.084753
N	-2.052564	-1.972863	3.22875
N	-1.223582	-0.889406	1.455707
N	-2.644597	-0.863568	1.414289
C	-3.119744	-1.519286	2.487446
H	-4.158124	-1.682505	2.755527
C	-0.909124	-1.568185	2.565993
H	0.075883	-1.797678	2.940783
Fe	3.588857	-0.002192	0.000422
N	2.05181	1.809937	3.323069
N	1.222923	0.815993	1.498272
N	2.643916	0.791395	1.45619
C	3.119023	1.392921	2.560672
H	4.157373	1.542119	2.836917

Atom	X	Y	Z
C	0.908406	1.439195	2.640684
H	-0.076583	1.650559	3.026033
N	2.04907	-3.784511	-0.094143
N	1.221331	-1.706797	-0.042421
N	2.642312	-1.658843	-0.041328
C	3.116759	-2.916383	-0.072609
H	4.154935	-3.230853	-0.080558
C	0.906071	-3.007569	-0.07456
H	-0.079146	-3.446396	-0.085132
N	2.052591	1.972948	-3.228605
N	1.223599	0.889423	-1.455604
N	2.644645	0.863587	-1.41418
C	3.119772	1.519319	-2.487334
H	4.15815	1.68257	-2.755405
C	0.909154	1.568277	-2.565845
H	-0.075851	1.797871	-2.940584
N	2.042345	2.477531	4.546935
H	2.281233	1.926687	5.370366
H	2.284059	3.467404	4.530065
N	2.038874	-5.178188	-0.128673
H	2.277881	-5.615589	-1.017551
H	2.280064	-5.659044	0.736864
N	-2.042236	-2.477129	-4.547112
H	-2.282883	-3.467264	-4.530362
H	-2.282141	-1.926332	-5.370279
N	-2.03905	5.178146	0.127775
H	-2.282163	5.658607	-0.737447
H	-2.27618	5.615916	1.016976
N	-2.043099	-2.700001	4.418207
H	-2.282891	-2.19064	5.267674
H	-2.284043	-3.688014	4.352373
N	2.043136	2.700199	-4.417993
H	2.284334	3.688147	-4.352104
H	2.282636	2.190853	-5.26755

Table S3. Calculated bond lengths [Å] and angles [°] for the polymeric ionic $Fe(NH_2\text{-trz})_3^{2+}$ complex, in the LS state, containing three Fe atoms and six NH_2-trz ligands at the B3LYP/LanL2DZ/6-31+G* level of approximation

No	Parameter	B3LYP	No	Parameter	B3LYP
r1	r(1,4)	2.0991	τ16	τ(18,1,11,15)	135.3025
r2	r(1,11)	2.0992	τ17	τ(26,1,11,12)	-135.2558
r3	r(1,18)	2.0993	τ18	τ(26,1,11,15)	44.7708
r4	r(1,26)	2.0991	τ19	τ(40,1,11,12)	135.2765
r5	r(1,33)	2.0992	τ20	τ(40,1,11,15)	-44.697
r6	r(1,40)	2.0993	τ21	τ(12,11,33,34)	-180.0003
r7	r(2,5)	1.9084	τ22	τ(12,11,33,37)	-0.0087
r8	r(2,12)	1.9085	τ23	τ(15,11,33,34)	0.026
r9	r(2,19)	1.9085	τ24	τ(15,11,33,37)	-179.9824
r10	r(3,6)	1.3763	τ25	τ(4,1,18,19)	-44.763
r11	r(3,8)	1.3822	τ26	τ(4,1,18,22)	135.2396
r12	r(3,52)	1.3941	τ27	τ(11,1,18,19)	44.7579
r13	r(4,5)	1.4218	τ28	τ(11,1,18,22)	-135.2395
r14	r(4,8)	1.3388	τ29	τ(26,1,18,19)	135.2376
r15	r(5,6)	1.3444	τ30	τ(26,1,18,22)	-44.7598
r16	r(6,7)	1.0848	τ31	τ(33,1,18,19)	-135.2416
r17	r(8,9)	1.0786	τ32	τ(33,1,18,22)	44.761
r18	r(10,13)	1.3763	τ33	τ(19,18,40,41)	179.9997
r19	r(10,15)	1.3822	τ34	τ(19,18,40,44)	0.0016
r20	r(10,55)	1.3941	τ35	τ(22,18,40,41)	0.003
r21	r(11,12)	1.4218	τ36	τ(22,18,40,44)	-179.9951
r22	r(11,15)	1.3388	τ37	τ(11,1,26,27)	-135.2929
r23	r(12,13)	1.3444	τ38	τ(11,1,26,30)	44.7294
r24	r(13,14)	1.0848	τ39	τ(18,1,26,27)	135.2006
r25	r(15,16)	1.0786	τ40	τ(18,1,26,30)	-44.777
r26	r(17,20)	1.3763	τ41	τ(33,1,26,27)	44.7081
r27	r(17,22)	1.3822	τ42	τ(33,1,26,30)	-135.2695
r28	r(17,58)	1.3941	τ43	τ(40,1,26,27)	-44.8001
r29	r(18,19)	1.4219	τ44	τ(40,1,26,30)	135.2223

No	Parameter	B3LYP	No	Parameter	B3LYP
r30	r(18,22)	1.3388	τ45	τ(4,1,33,34)	135.254
r31	r(19,20)	1.3444	τ46	τ(4,1,33,37)	-44.7541
r32	r(20,21)	1.0848	τ47	τ(18,1,33,34)	-135.2764
r33	r(22,23)	1.0786	τ48	τ(18,1,33,37)	44.7154
r34	r(24,27)	1.9084	τ49	τ(26,1,33,34)	-44.7447
r35	r(24,34)	1.9085	τ50	τ(26,1,33,37)	135.2471
r36	r(24,41)	1.9085	τ51	τ(40,1,33,34)	44.723
r37	r(25,28)	1.3763	τ52	τ(40,1,33,37)	-135.2852
r38	r(25,30)	1.3822	τ53	τ(4,1,40,41)	-135.2367
r39	r(25,46)	1.3941	τ54	τ(4,1,40,44)	44.7645
r40	r(26,27)	1.4218	τ55	τ(11,1,40,41)	135.2425
r41	r(26,30)	1.3388	τ56	τ(11,1,40,44)	-44.7563
r42	r(27,28)	1.3444	τ57	τ(26,1,40,41)	44.7627
r43	r(28,29)	1.0848	τ58	τ(26,1,40,44)	-135.2361
r44	r(30,31)	1.0786	τ59	τ(33,1,40,41)	-44.7581
r45	r(32,35)	1.3763	τ60	τ(33,1,40,44)	135.2431
r46	r(32,37)	1.3822	τ61	τ(12,2,5,4)	49.381
r47	r(32,49)	1.3941	τ62	τ(12,2,5,6)	-130.6474
r48	r(33,34)	1.4218	τ63	τ(19,2,5,4)	-49.3712
r49	r(33,37)	1.3388	τ64	τ(19,2,5,6)	130.6004
r50	r(34,35)	1.3444	τ65	τ(5,2,12,11)	-49.3461
r51	r(35,36)	1.0848	τ66	τ(5,2,12,13)	130.6153
r52	r(37,38)	1.0786	τ67	τ(19,2,12,11)	49.3914
r53	r(39,42)	1.3763	τ68	τ(19,2,12,13)	-130.6473
r54	r(39,44)	1.3822	τ69	τ(5,2,19,18)	49.3978
r55	r(39,61)	1.3941	τ70	τ(5,2,19,20)	-130.6273
r56	r(40,41)	1.4219	τ71	τ(12,2,19,18)	-49.3541
r57	r(40,44)	1.3388	τ72	τ(12,2,19,20)	130.6208
r58	r(41,42)	1.3444	τ73	τ(8,3,6,5)	-0.0043
r59	r(42,43)	1.0848	τ74	τ(8,3,6,7)	179.9939
r60	r(44,45)	1.0786	τ75	τ(52,3,6,5)	-180.0057
r61	r(46,47)	1.0191	τ76	τ(52,3,6,7)	-0.0074
r62	r(46,48)	1.0191	τ77	τ(6,3,8,4)	-0.0034

No	Parameter	B3LYP	No	Parameter	B3LYP
r63	r(49,50)	1.0191	τ78	τ(6,3,8,9)	179.9976
r64	r(49,51)	1.0191	τ79	τ(52,3,8,4)	179.9978
r65	r(52,53)	1.0191	τ80	τ(52,3,8,9)	-0.0011
r66	r(52,54)	1.0191	τ81	τ(6,3,52,53)	-74.5334
r67	r(55,56)	1.0191	τ82	τ(6,3,52,54)	74.4609
r68	r(55,57)	1.0191	τ83	τ(8,3,52,53)	105.4651
r69	r(58,59)	1.0191	τ84	τ(8,3,52,54)	-105.5406
r70	r(58,60)	1.0191	τ85	τ(1,4,5,2)	-0.0479
r71	r(61,62)	1.0191	τ86	τ(1,4,5,6)	179.9752
r72	r(61,63)	1.0191	τ87	τ(8,4,5,2)	179.965
α1	α(4,1,11)	89.5162	τ88	τ(8,4,5,6)	-0.0119
α2	α(4,1,18)	89.4654	τ89	τ(1,4,8,3)	-179.9766
α3	α(4,1,33)	90.4832	τ90	τ(1,4,8,9)	0.0223
α4	α(4,1,40)	90.5352	τ91	τ(5,4,8,3)	0.0093
α5	α(11,1,18)	89.5019	τ92	τ(5,4,8,9)	-179.9919
α6	α(11,1,26)	90.4844	τ93	τ(2,5,6,3)	-179.9644
α7	α(11,1,40)	90.4974	τ94	τ(2,5,6,7)	0.0374
α8	α(18,1,26)	90.5358	τ95	τ(4,5,6,3)	0.0101
α9	α(18,1,33)	90.497	τ96	τ(4,5,6,7)	-179.9881
α10	α(26,1,33)	89.5162	τ97	τ(15,10,13,12)	0.0059
α11	α(26,1,40)	89.4636	τ98	τ(15,10,13,14)	179.9983
α12	α(33,1,40)	89.5037	τ99	τ(55,10,13,12)	179.9727
α13	α(5,2,12)	97.5907	τ100	τ(55,10,13,14)	-0.0349
α14	α(5,2,19)	97.574	τ101	τ(13,10,15,11)	-0.0155
α15	α(12,2,19)	97.591	τ102	τ(13,10,15,16)	179.982
α16	α(6,3,8)	106.6612	τ103	τ(55,10,15,11)	-179.9847
α17	α(6,3,52)	129.5435	τ104	τ(55,10,15,16)	0.0129
α18	α(8,3,52)	123.7953	τ105	τ(13,10,55,56)	-74.289
α19	α(1,4,5)	123.6699	τ106	τ(13,10,55,57)	74.6972
α20	α(1,4,8)	130.7788	τ107	τ(15,10,55,56)	105.6727
α21	α(5,4,8)	105.5512	τ108	τ(15,10,55,57)	-105.3411
α22	α(2,5,4)	121.6443	τ109	τ(1,11,12,2)	-0.0249
α23	α(2,5,6)	129.6241	τ110	τ(1,11,12,13)	180.0065

No	Parameter	B3LYP	No	Parameter	B3LYP
α24	α(4,5,6)	108.7316	τ111	τ(15,11,12,2)	179.9542
α25	α(3,6,5)	108.4593	τ112	τ(15,11,12,13)	-0.0143
α26	α(3,6,7)	124.0217	τ113	τ(1,11,15,10)	-180.0048
α27	α(5,6,7)	127.519	τ114	τ(1,11,15,16)	-0.0021
α28	α(3,8,4)	110.5967	τ115	τ(12,11,15,10)	0.0182
α29	α(3,8,9)	121.7687	τ116	τ(12,11,15,16)	-179.9792
α30	α(4,8,9)	127.6346	τ117	τ(2,12,13,10)	-179.9602
α31	α(13,10,15)	106.6632	τ118	τ(2,12,13,14)	0.0478
α32	α(13,10,55)	129.5427	τ119	τ(11,12,13,10)	0.0051
α33	α(15,10,55)	123.7941	τ120	τ(11,12,13,14)	-179.987
α34	α(1,11,12)	123.6433	τ121	τ(22,17,20,19)	0.0038
α35	α(1,11,15)	130.8032	τ122	τ(22,17,20,21)	-179.987
α36	α(12,11,15)	105.5535	τ123	τ(58,17,20,19)	180.0054
α37	α(2,12,11)	121.6696	τ124	τ(58,17,20,21)	0.0146
α38	α(2,12,13)	129.5983	τ125	τ(20,17,22,18)	-0.002
α39	α(11,12,13)	108.7321	τ126	τ(20,17,22,23)	-180.0003
α40	α(10,13,12)	108.4575	τ127	τ(58,17,22,18)	-180.0034
α41	α(10,13,14)	124.0203	τ128	τ(58,17,22,23)	-0.0018
α42	α(12,13,14)	127.5222	τ129	τ(20,17,58,59)	-74.5112
α43	α(10,15,11)	110.5937	τ130	τ(20,17,58,60)	74.4728
α44	α(10,15,16)	121.7716	τ131	τ(22,17,58,59)	105.4906
α45	α(11,15,16)	127.6347	τ132	τ(22,17,58,60)	-105.5254
α46	α(20,17,22)	106.6609	τ133	τ(1,18,19,2)	-0.0154
α47	α(20,17,58)	129.5466	τ134	τ(1,18,19,20)	-179.995
α48	α(22,17,58)	123.7924	τ135	τ(22,18,19,2)	179.9825
α49	α(1,18,19)	123.6838	τ136	τ(22,18,19,20)	0.0029
α50	α(1,18,22)	130.7641	τ137	τ(1,18,22,17)	179.9972
α51	α(19,18,22)	105.5522	τ138	τ(1,18,22,23)	-0.0045
α52	α(2,19,18)	121.6228	τ139	τ(19,18,22,17)	-0.0005
α53	α(2,19,20)	129.6475	τ140	τ(19,18,22,23)	179.9977
α54	α(18,19,20)	108.7297	τ141	τ(2,19,20,17)	-179.9816
α55	α(17,20,19)	108.4605	τ142	τ(2,19,20,21)	0.0087
α56	α(17,20,21)	124.0244	τ143	τ(18,19,20,17)	-0.0042

No	Parameter	B3LYP	No	Parameter	B3LYP
α57	α(19,20,21)	127.5151	τ144	τ(18,19,20,21)	179.9862
α58	α(17,22,18)	110.5967	τ145	τ(34,24,27,26)	-49.3872
α59	α(17,22,23)	121.7741	τ146	τ(34,24,27,28)	130.6543
α60	α(18,22,23)	127.6292	τ147	τ(41,24,27,26)	49.3706
α61	α(27,24,34)	97.5898	τ148	τ(41,24,27,28)	-130.5879
α62	α(27,24,41)	97.5738	τ149	τ(27,24,34,33)	49.349
α63	α(34,24,41)	97.5967	τ150	τ(27,24,34,35)	-130.6228
α64	α(28,25,30)	106.6612	τ151	τ(41,24,34,33)	-49.389
α65	α(28,25,46)	129.5437	τ152	τ(41,24,34,35)	130.6392
α66	α(30,25,46)	123.7951	τ153	τ(27,24,41,40)	-49.4025
α67	α(1,26,27)	123.6702	τ154	τ(27,24,41,42)	130.6285
α68	α(1,26,30)	130.779	τ155	τ(34,24,41,40)	49.3494
α69	α(27,26,30)	105.5508	τ156	τ(34,24,41,42)	-130.6196
α70	α(24,27,26)	121.6434	τ157	τ(30,25,28,27)	0.0075
α71	α(24,27,28)	129.6253	τ158	τ(30,25,28,29)	-179.9889
α72	α(26,27,28)	108.7313	τ159	τ(46,25,28,27)	-179.9832
α73	α(25,28,27)	108.4596	τ160	τ(46,25,28,29)	0.0204
α74	α(25,28,29)	124.022	τ161	τ(28,25,30,26)	-0.0056
α75	α(27,28,29)	127.5184	τ162	τ(28,25,30,31)	-179.9972
α76	α(25,30,26)	110.5971	τ163	τ(46,25,30,26)	179.9857
α77	α(25,30,31)	121.7691	τ164	τ(46,25,30,31)	-0.0058
α78	α(26,30,31)	127.6338	τ165	τ(28,25,46,47)	-74.5343
α79	α(35,32,37)	106.6632	τ166	τ(28,25,46,48)	74.4578
α80	α(35,32,49)	129.5419	τ167	τ(30,25,46,47)	105.4764
α81	α(37,32,49)	123.7949	τ168	τ(30,25,46,48)	-105.5315
α82	α(1,33,34)	123.6448	τ169	τ(1,26,27,24)	0.0544
α83	α(1,33,37)	130.8022	τ170	τ(1,26,27,28)	-179.9793
α84	α(34,33,37)	105.553	τ171	τ(30,26,27,24)	-179.9632
α85	α(24,34,33)	121.6674	τ172	τ(30,26,27,28)	0.0031
α86	α(24,34,35)	129.6011	τ173	τ(1,26,30,25)	179.9823
α87	α(33,34,35)	108.7314	τ174	τ(1,26,30,31)	-0.0268
α88	α(32,35,34)	108.4581	τ175	τ(27,26,30,25)	0.0016
α89	α(32,35,36)	124.0202	τ176	τ(27,26,30,31)	179.9926

No	Parameter	B3LYP	No	Parameter	B3LYP
α90	α(34,35,36)	127.5217	τ177	τ(24,27,28,25)	179.9561
α91	α(32,37,33)	110.5942	τ178	τ(24,27,28,29)	-0.0477
α92	α(32,37,38)	121.7712	τ179	τ(26,27,28,25)	-0.0066
α93	α(33,37,38)	127.6346	τ180	τ(26,27,28,29)	179.9896
α94	α(42,39,44)	106.661	τ181	τ(37,32,35,34)	-0.0095
α95	α(42,39,61)	129.5462	τ182	τ(37,32,35,36)	179.9961
α96	α(44,39,61)	123.7928	τ183	τ(49,32,35,34)	-179.994
α97	α(1,40,41)	123.6836	τ184	τ(49,32,35,36)	0.0116
α98	α(1,40,44)	130.7647	τ185	τ(35,32,37,33)	0.0144
α99	α(41,40,44)	105.5518	τ186	τ(35,32,37,38)	-179.9845
α100	α(24,41,40)	121.621	τ187	τ(49,32,37,33)	-180
α101	α(24,41,42)	129.6503	τ188	τ(49,32,37,38)	0.001
α102	α(40,41,42)	108.7287	τ189	τ(35,32,49,50)	-74.566
α103	α(39,42,41)	108.4614	τ190	τ(35,32,49,51)	74.4212
α104	α(39,42,43)	124.024	τ191	τ(37,32,49,50)	105.4519
α105	α(41,42,43)	127.5146	τ192	τ(37,32,49,51)	-105.561
α106	α(39,44,40)	110.5972	τ193	τ(1,33,34,24)	0.0236
α107	α(39,44,45)	121.7736	τ194	τ(1,33,34,35)	-179.9993
α108	α(40,44,45)	127.6292	τ195	τ(37,33,34,24)	-179.97
α109	α(25,46,47)	116.6729	τ196	τ(37,33,34,35)	0.0071
α110	α(25,46,48)	116.6785	τ197	τ(1,33,37,32)	179.9939
α111	α(47,46,48)	118.8686	τ198	τ(1,33,37,38)	-0.0072
α112	α(32,49,50)	116.6764	τ199	τ(34,33,37,32)	-0.0132
α113	α(32,49,51)	116.6746	τ200	τ(34,33,37,38)	179.9857
α114	α(50,49,51)	118.8667	τ201	τ(24,34,35,32)	179.9763
α115	α(3,52,53)	116.6789	τ202	τ(24,34,35,36)	-0.0296
α116	α(3,52,54)	116.6733	τ203	τ(33,34,35,32)	0.0016
α117	α(53,52,54)	118.869	τ204	τ(33,34,35,36)	179.9958
α118	α(10,55,56)	116.6743	τ205	τ(44,39,42,41)	-0.0045
α119	α(10,55,57)	116.6769	τ206	τ(44,39,42,43)	179.9903
α120	α(56,55,57)	118.8661	τ207	τ(61,39,42,41)	179.9894
α121	α(17,58,59)	116.6723	τ208	τ(61,39,42,43)	-0.0158
α122	α(17,58,60)	116.6756	τ209	τ(42,39,44,40)	0.0005

No	Parameter	B3LYP	No	Parameter	B3LYP
α123	α(59,58,60)	118.8679	τ210	τ(42,39,44,45)	179.996
α124	α(39,61,62)	116.6758	τ211	τ(61,39,44,40)	180.0061
α125	α(39,61,63)	116.6727	τ212	τ(61,39,44,45)	0.0016
α126	α(62,61,63)	118.8687	τ213	τ(42,39,61,62)	-74.4552
τ1	τ(11,1,4,5)	-44.7121	τ214	τ(42,39,61,63)	74.5317
τ2	τ(11,1,4,8)	135.2715	τ215	τ(44,39,61,62)	105.5378
τ3	τ(18,1,4,5)	44.7943	τ216	τ(44,39,61,63)	-105.4753
τ4	τ(18,1,4,8)	-135.2221	τ217	τ(1,40,41,24)	0.0199
τ5	τ(33,1,4,5)	135.2868	τ218	τ(1,40,41,42)	179.9946
τ6	τ(33,1,4,8)	-44.7296	τ219	τ(44,40,41,24)	-179.9811
τ7	τ(40,1,4,5)	-135.205	τ220	τ(44,40,41,42)	-0.0063
τ8	τ(40,1,4,8)	44.7786	τ221	τ(1,40,44,39)	-179.9976
τ9	τ(5,4,26,27)	179.9952	τ222	τ(1,40,44,45)	0.0072
τ10	τ(5,4,26,30)	0.0172	τ223	τ(41,40,44,39)	0.0035
τ11	τ(8,4,26,27)	-0.0215	τ224	τ(41,40,44,45)	-179.9917
τ12	τ(8,4,26,30)	180.0005	τ225	τ(24,41,42,39)	179.9788
τ13	τ(4,1,11,12)	44.7455	τ226	τ(24,41,42,43)	-0.0157
τ14	τ(4,1,11,15)	-135.228	τ227	τ(40,41,42,39)	0.0067
τ15	τ(18,1,11,12)	-44.7241	τ228	τ(40,41,42,43)	-179.9878

r: Distances; α: Angle; τ:Dihedral angle