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An *N*-Tethered Uranium(III) Arene Complex and the Synthesis of an Unsupported U-Fe Bond

Skye Fortier,*[,†] J. Rolando Aguilar-Calderón,[†] Bess Vlaisavljevich,*[,‡] Alejandro J. Metta-Magaña,[†] Alan G. Goos,[⊥] and Cristian E. Botez[⊥]

†Department of Chemistry, University of Texas at El Paso, El Paso, Texas 79968, United States
‡Department of Chemistry, University of South Dakota, Vermillion, South Dakota 57069, United States
⊥ Department of Physics, University of Texas at El Paso, El Paso, Texas 79968, United States

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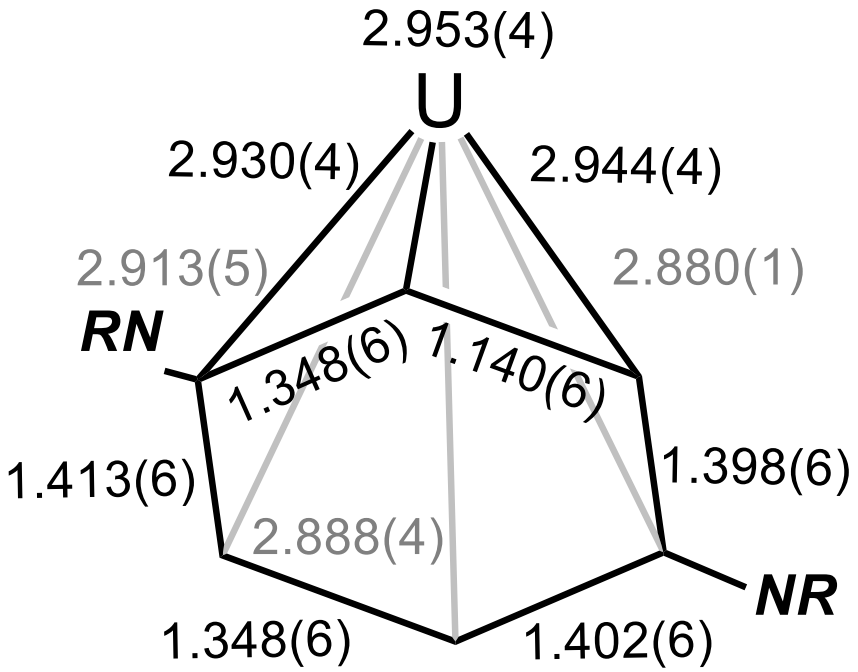

Figure S1. Pertinent bond length parameters from the solid-state molecular structure of **1**·DME.

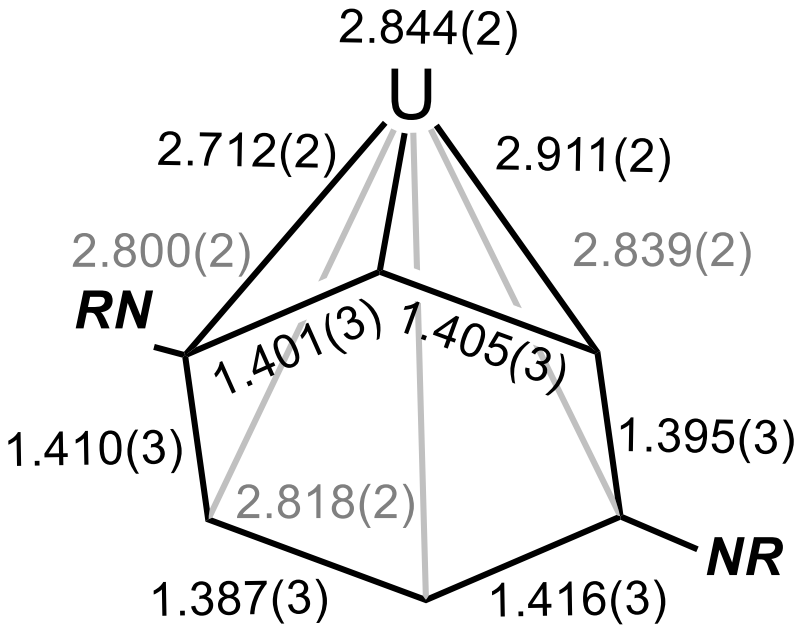

Figure S2. Pertinent bond length parameters from the solid-state molecular structure of **2**·0.5DME.

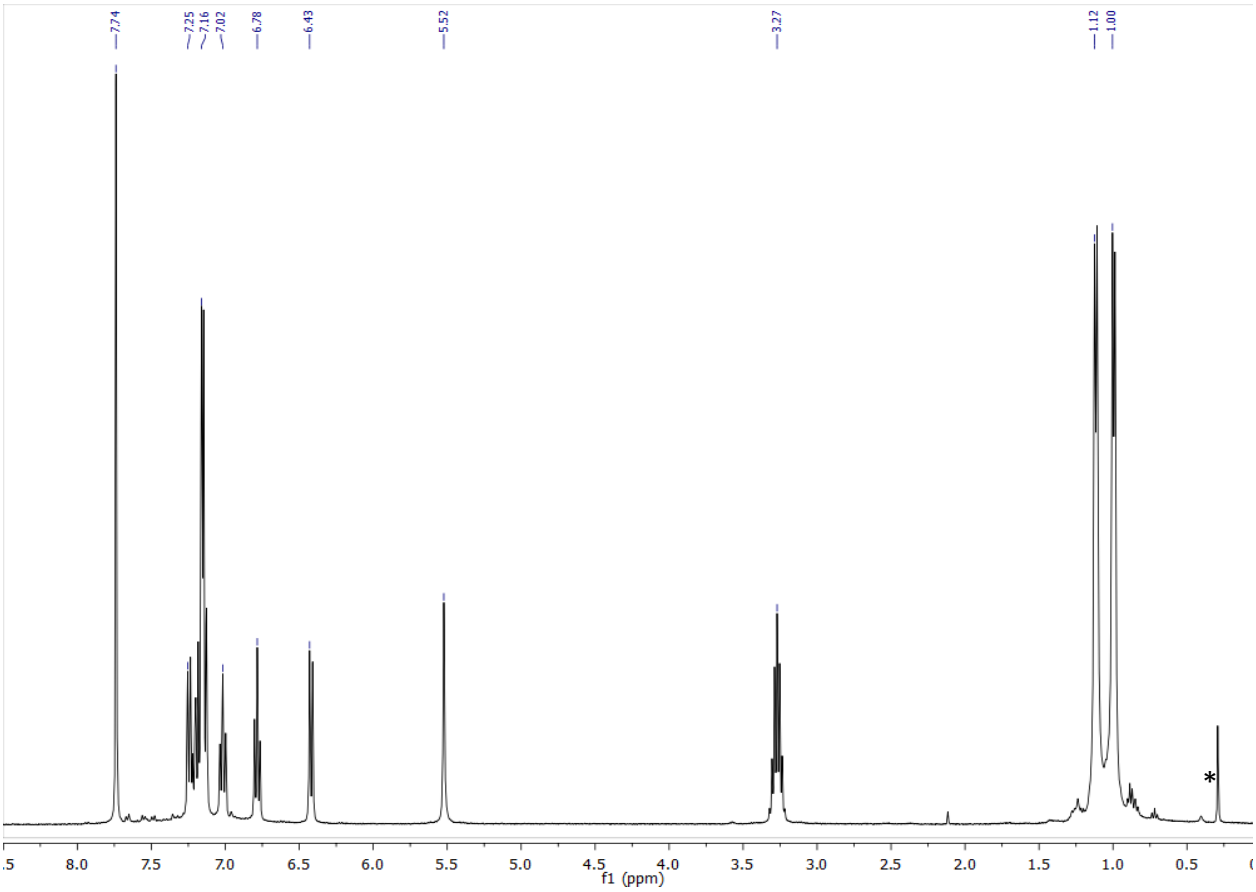

Figure S3. ^{1}H NMR spectrum of $\mathbf{H_2L^{Ar}}$ in C_6D_6. Resonance marked with asterisk denotes protons of residual silicon grease.

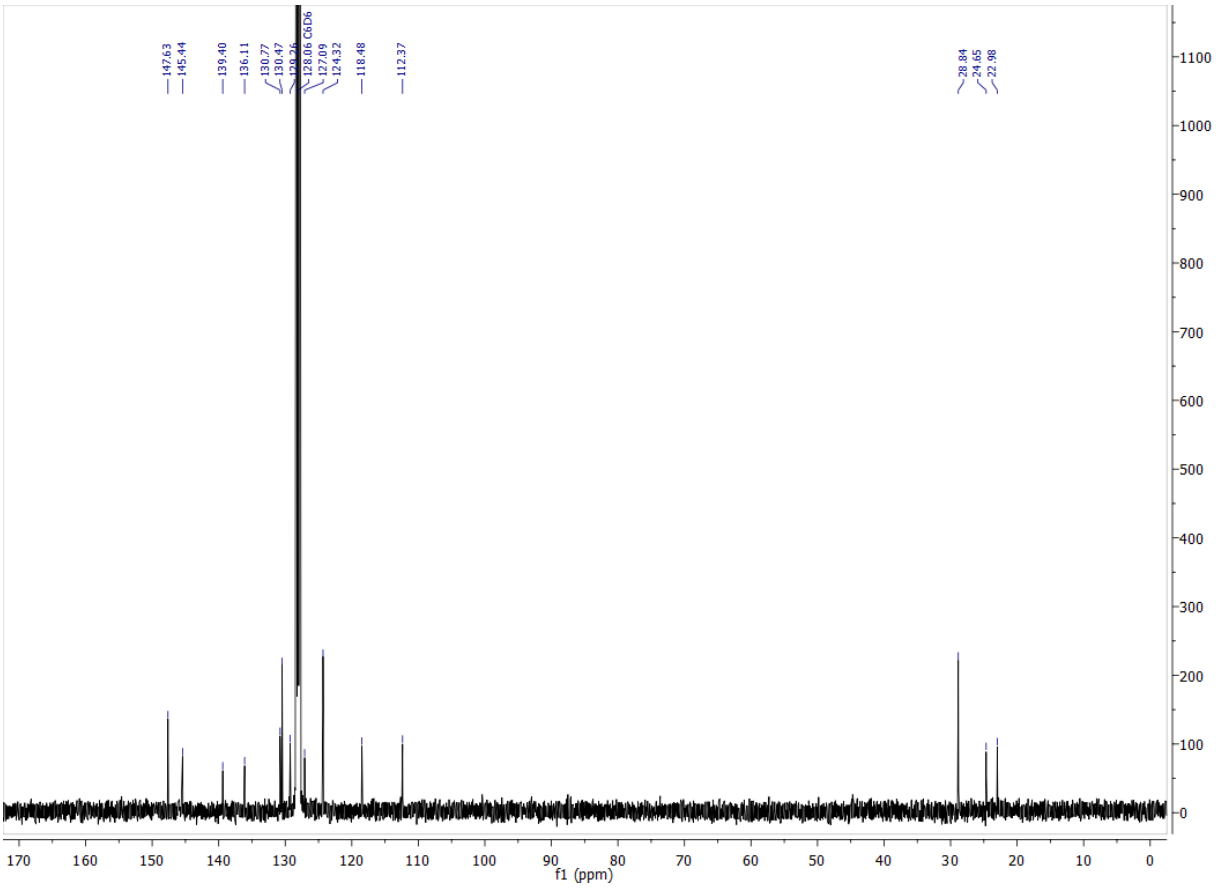

Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of $\mathbf{H_2L^{Ar}}$ in C_6D_6.

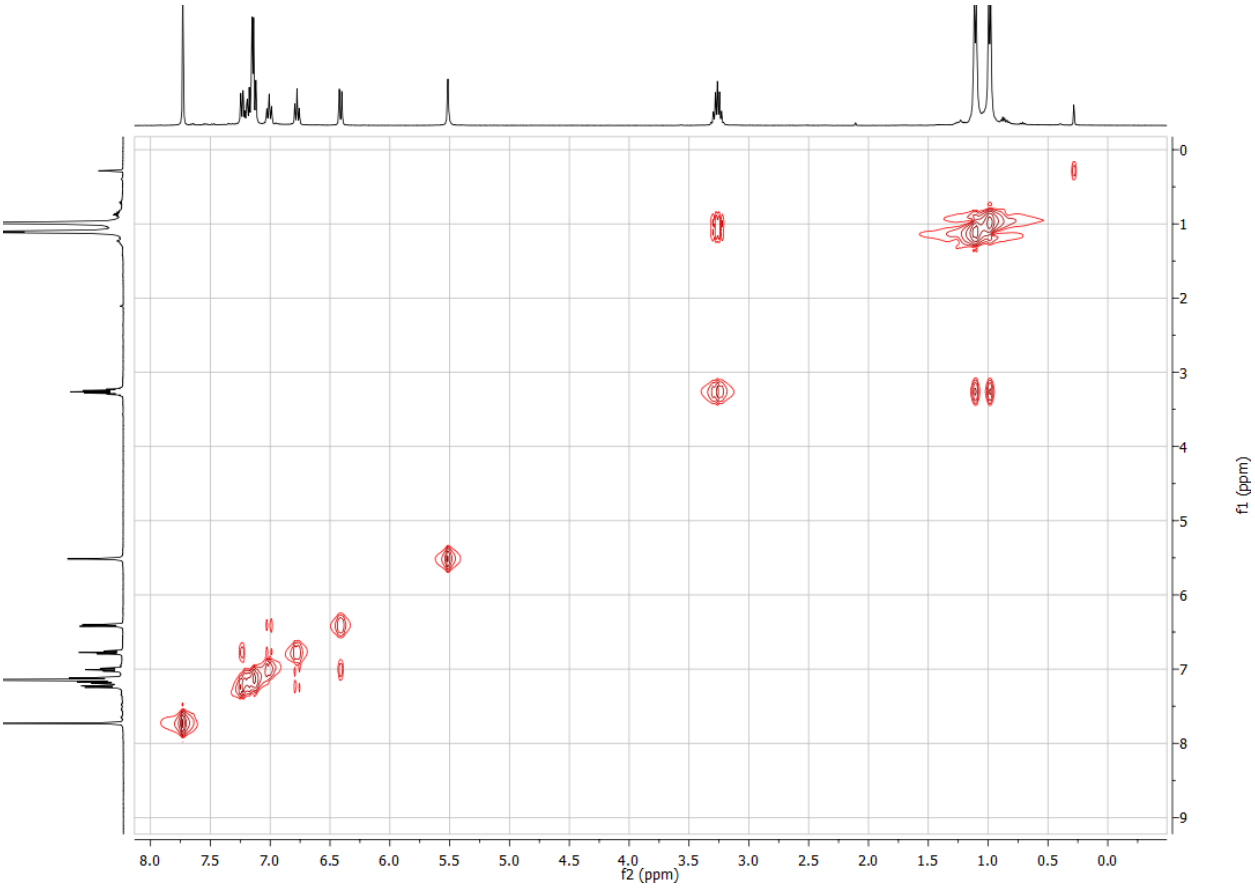

Figure S5. COSY NMR spectrum of $\mathbf{H_2L^{Ar}}$ in C_6D_6.

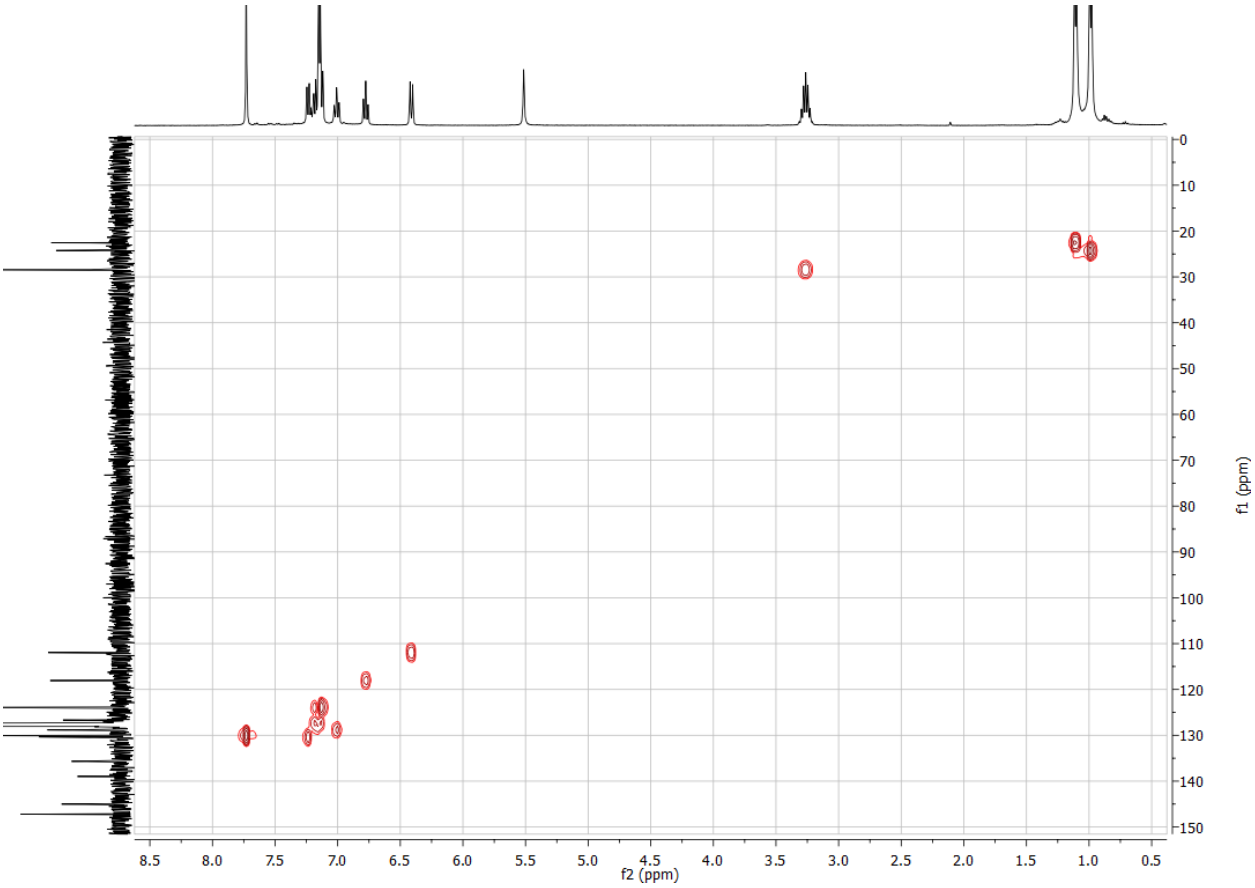

Figure S6. HMQC NMR spectrum of $\mathbf{H_2L^{Ar}}$ in C_6D_6.

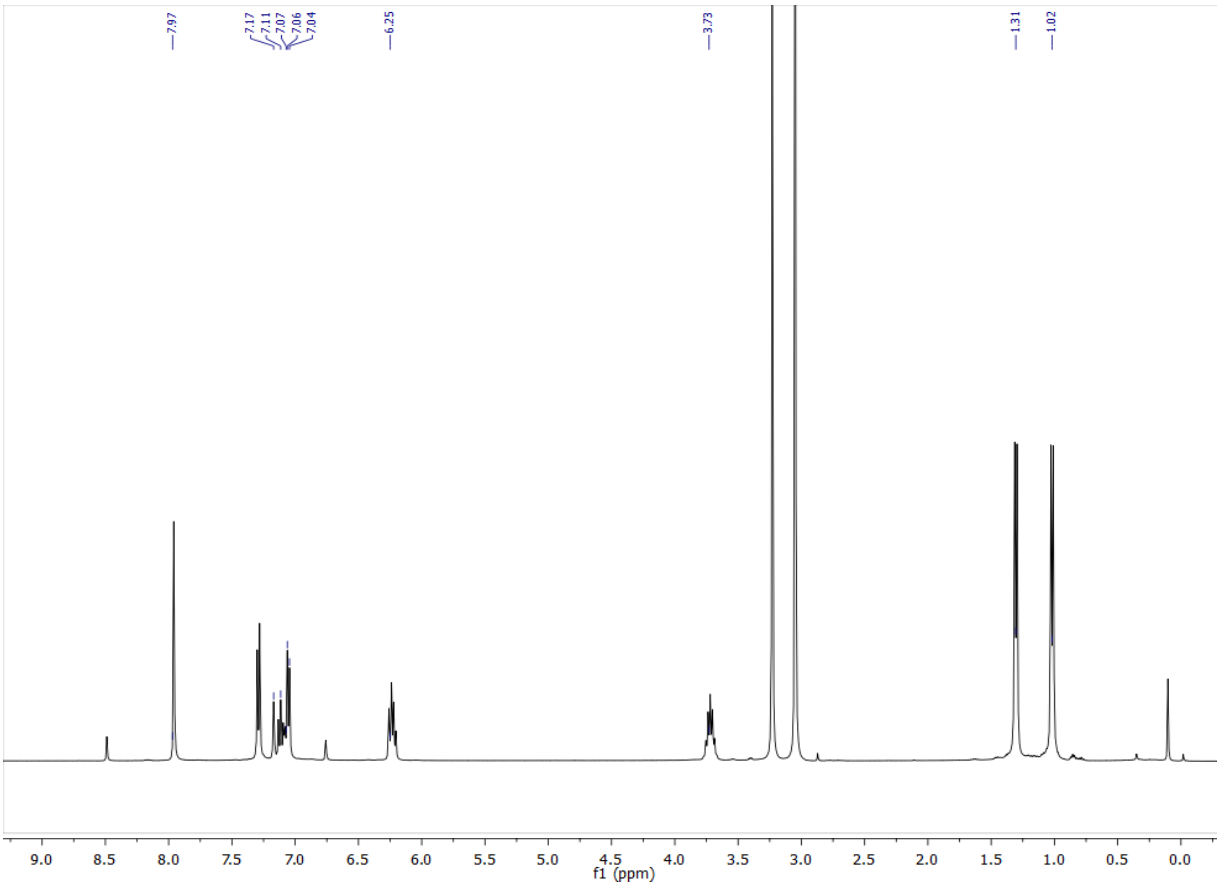

Figure S7. ^{1}H NMR spectrum of **[K(DME)$_2$]$_2$L^{Ar}** in C_6D_6/py-d_5 (10:1).

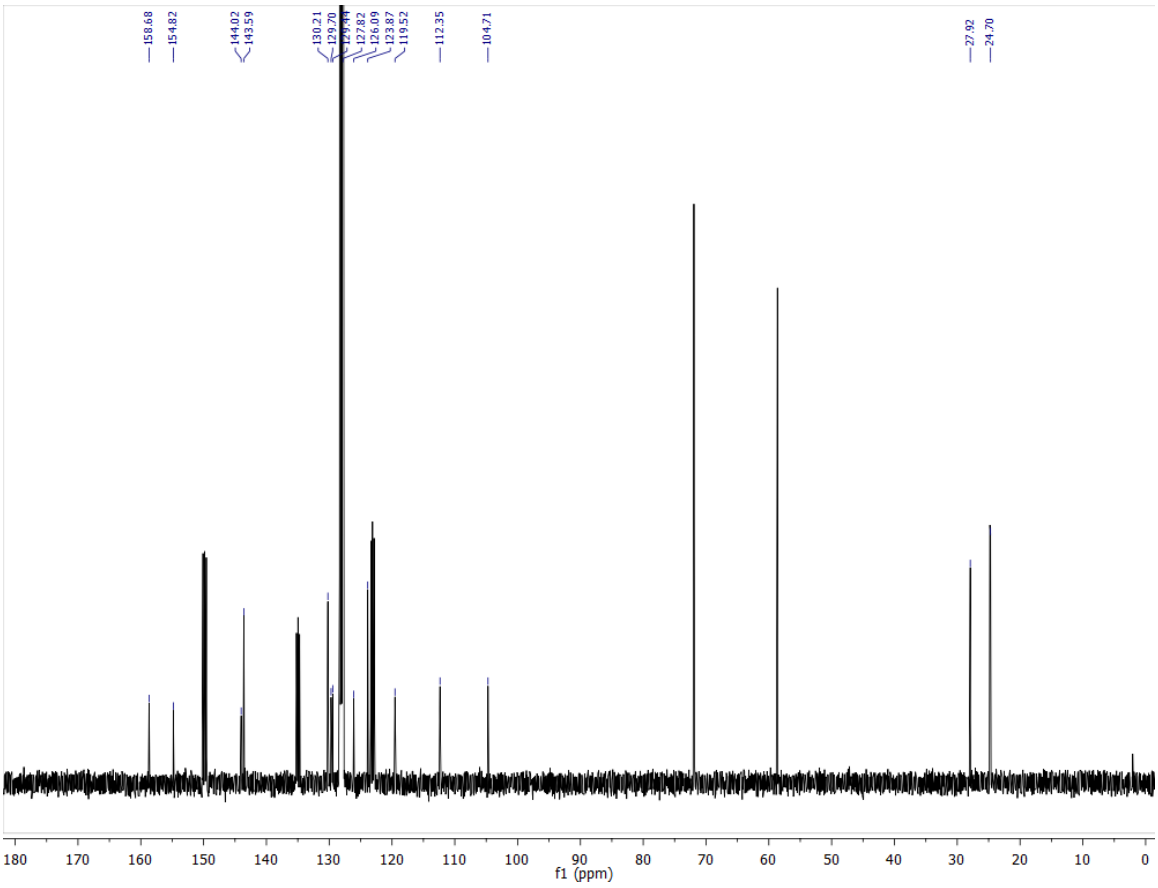

Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of **[K(DME)$_2$]$_2$L^{Ar}** in C_6D_6/py-d_5 (10:1).

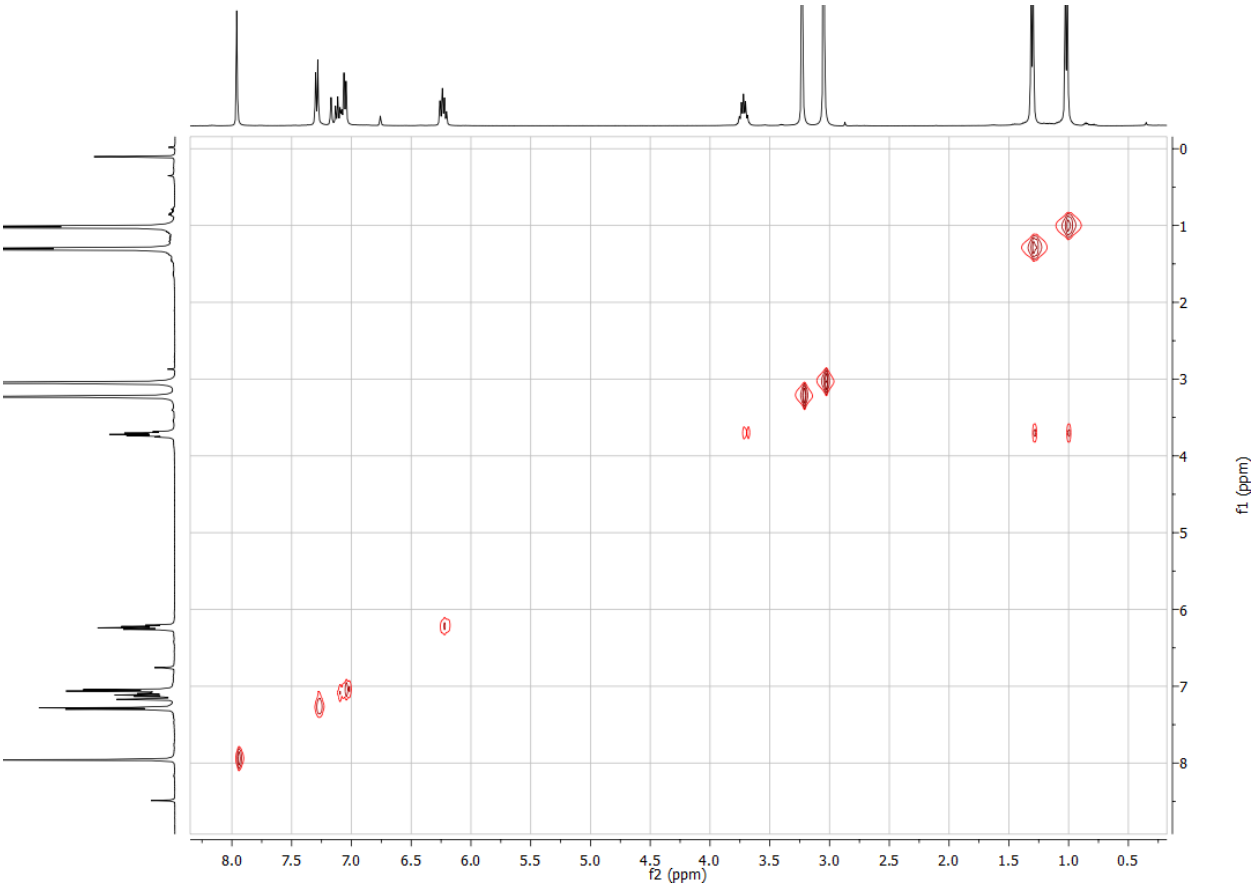

Figure S9. COSY ^{1}H NMR spectrum of **[K(DME)$_2$]$_2$L^{Ar}** in C_6D_6/py-d_5 (10:1)**..**

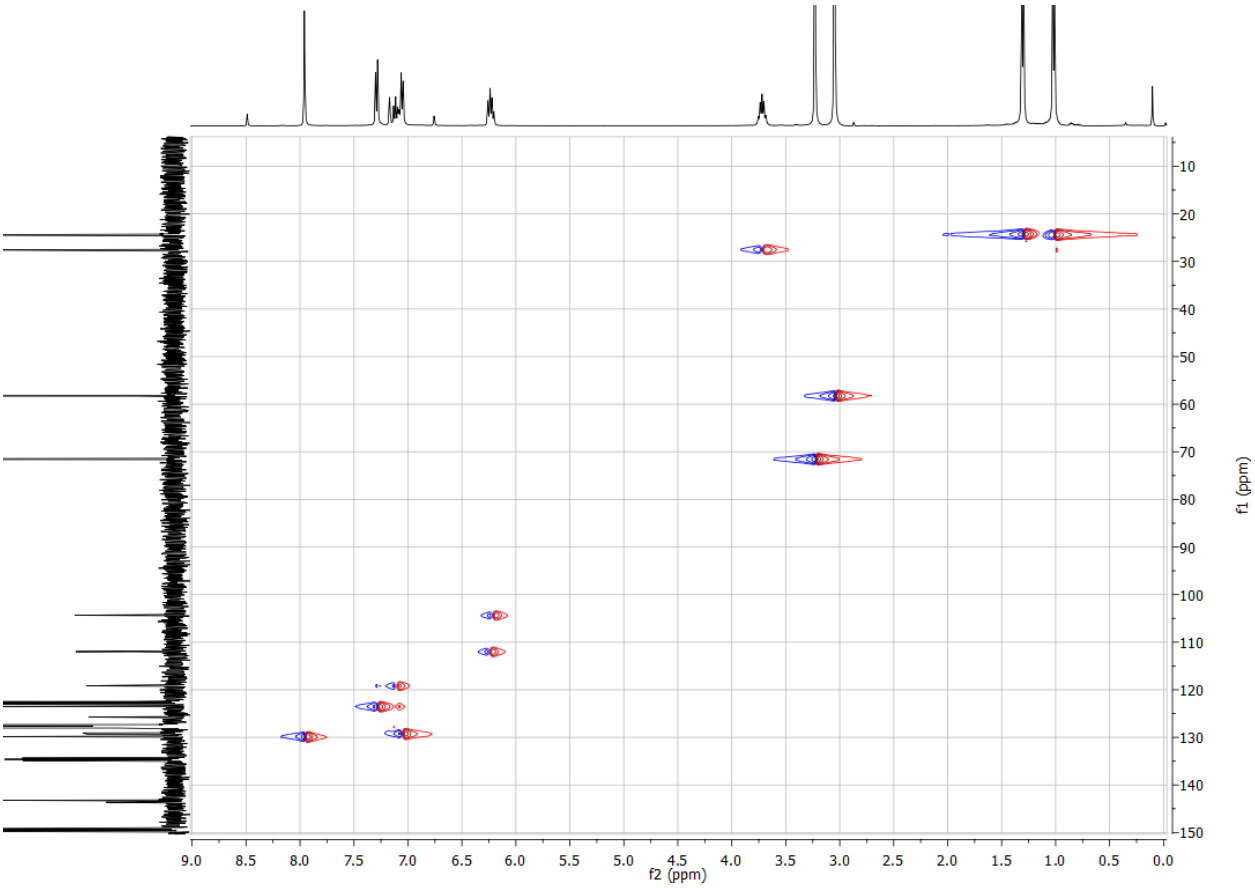

Figure S10. HSQC NMR spectrum of **[K(DME)$_2$]$_2$L^{Ar}** in C_6D_6/py-d_5 (10:1).

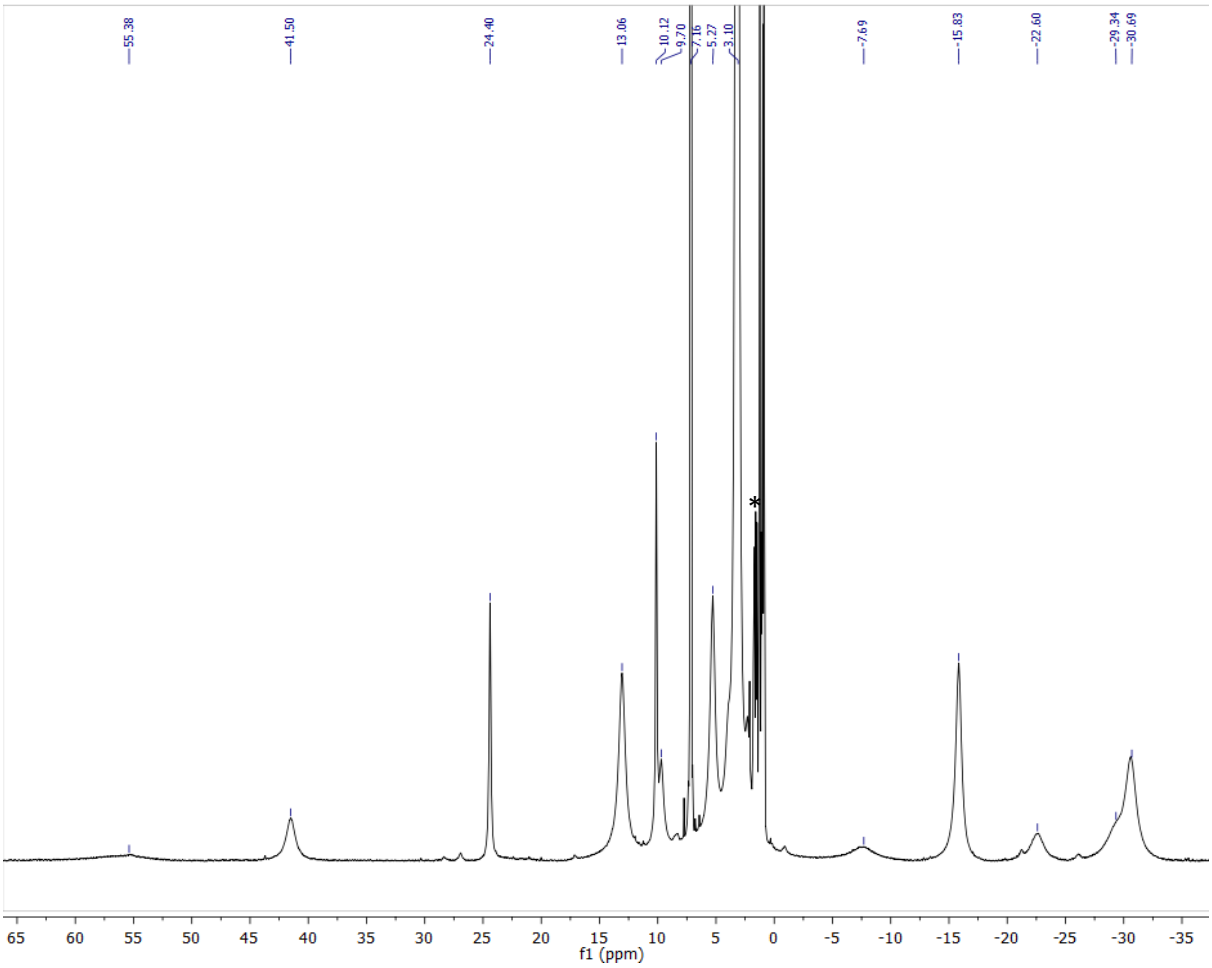

Figure S11. ^{1}H NMR spectrum of **1**•DME in C_6D_6. Resonances marked with asterisk denote protons of residual hexanes.

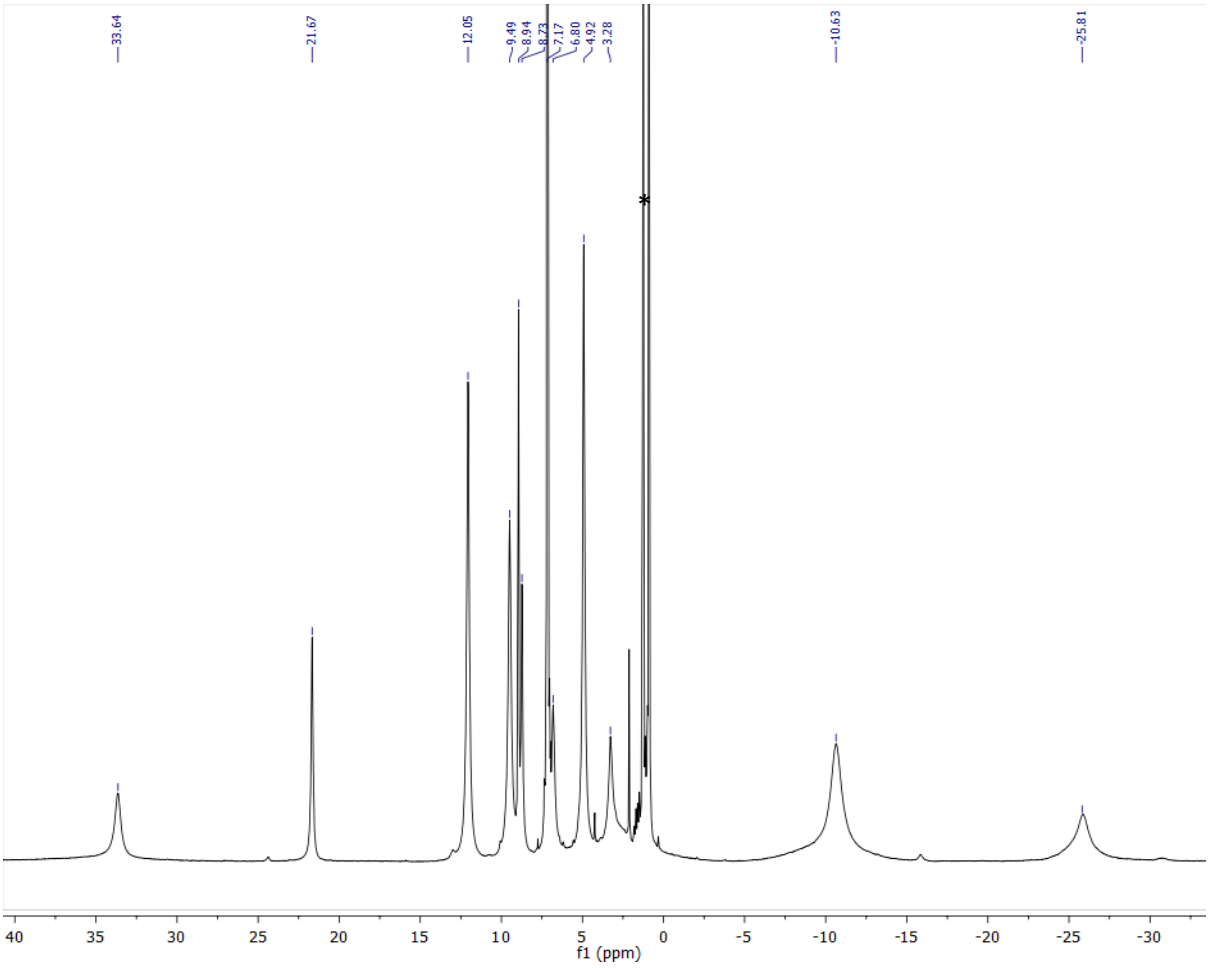

Figure S12. ^{1}H NMR spectrum of **2**•0.5DME. in C_6D_6. Resonances marked with asterisk denote protons of residual hexanes.

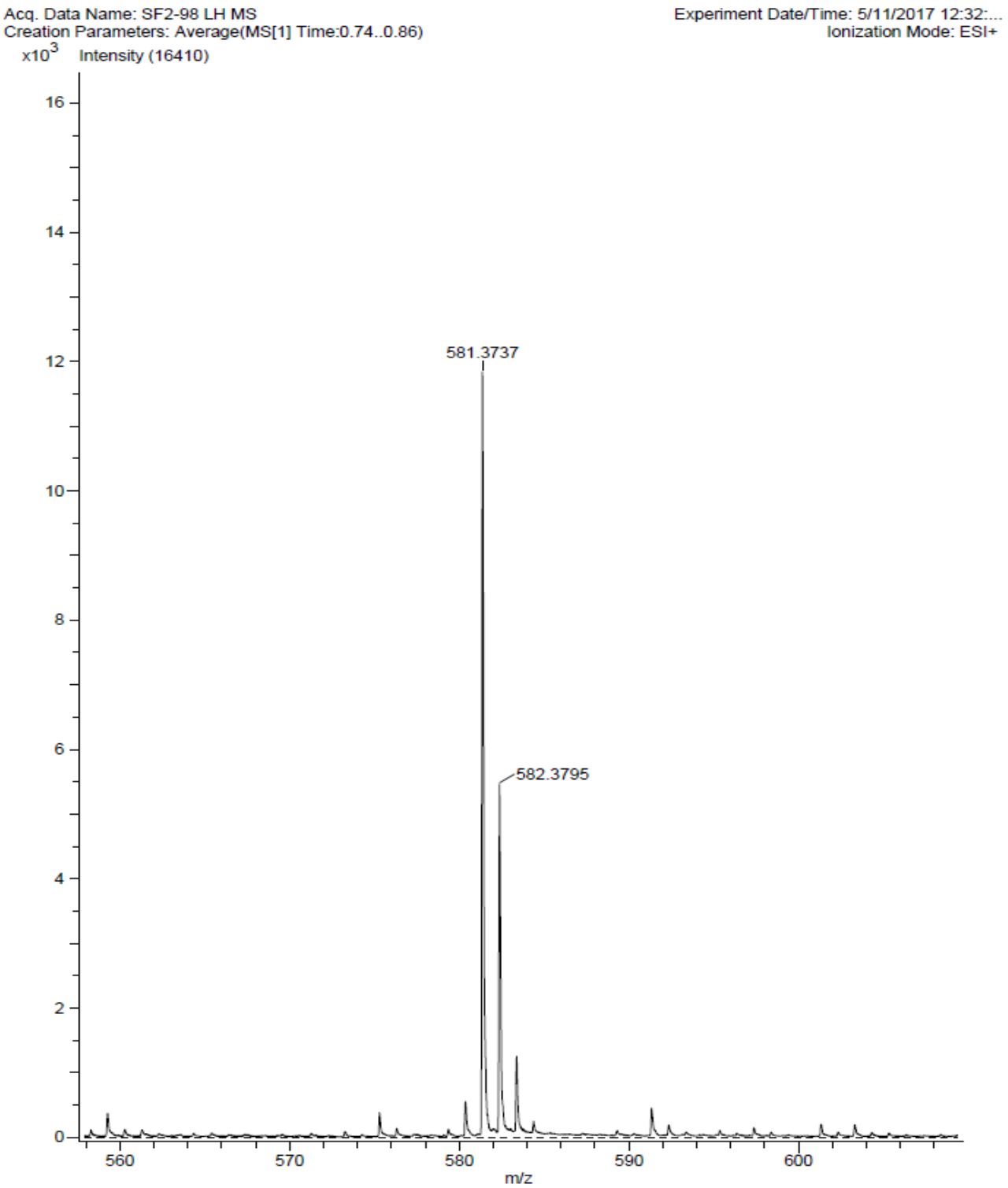

Figure S13. ESI mass spectrum of H_2L^{Ar}.

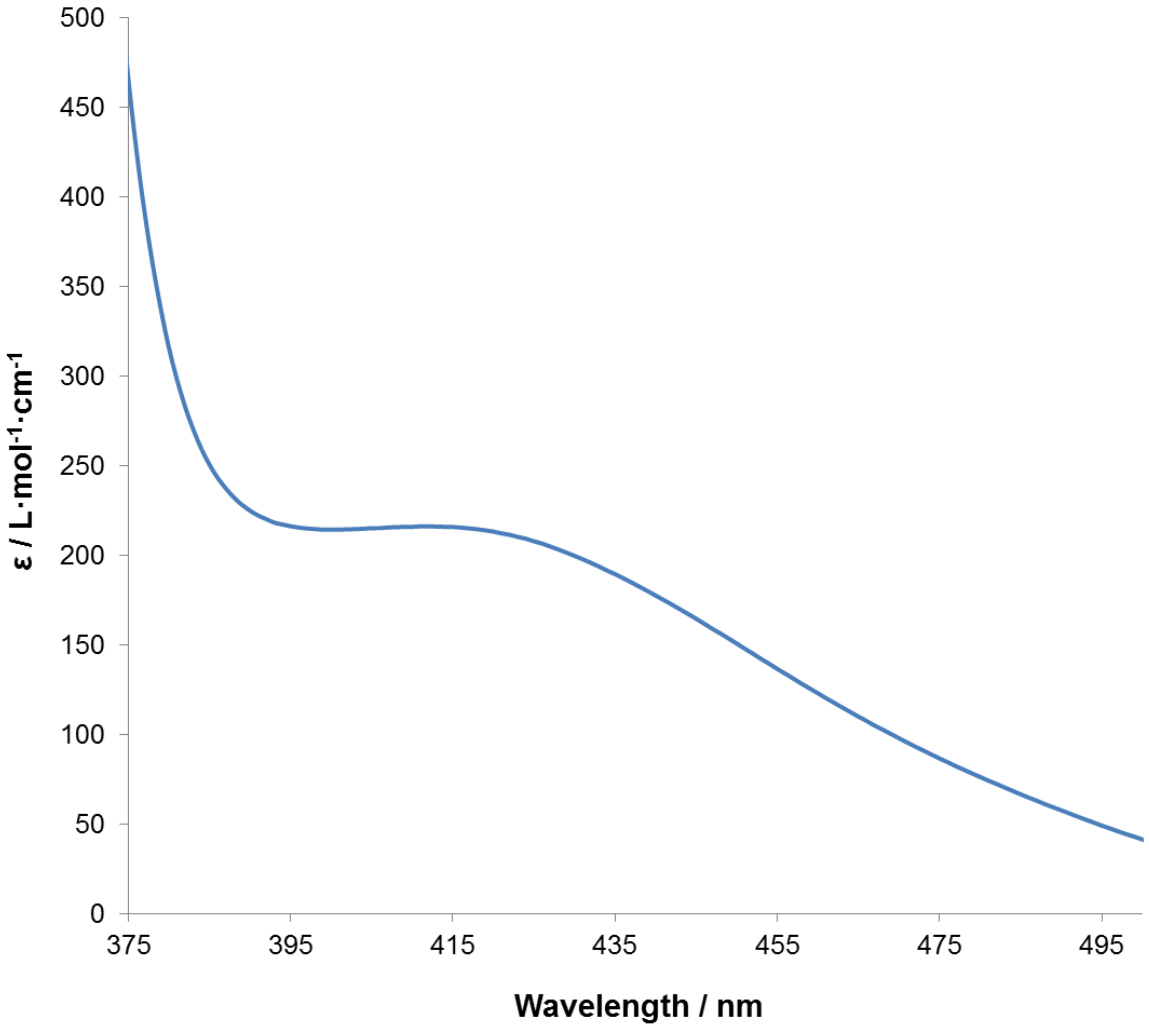

Figure S14. Room temperature UV/vis-NIR absorption spectra for $\mathbf{H_2L^{Ar}}$ (THF, 0.61 mM).

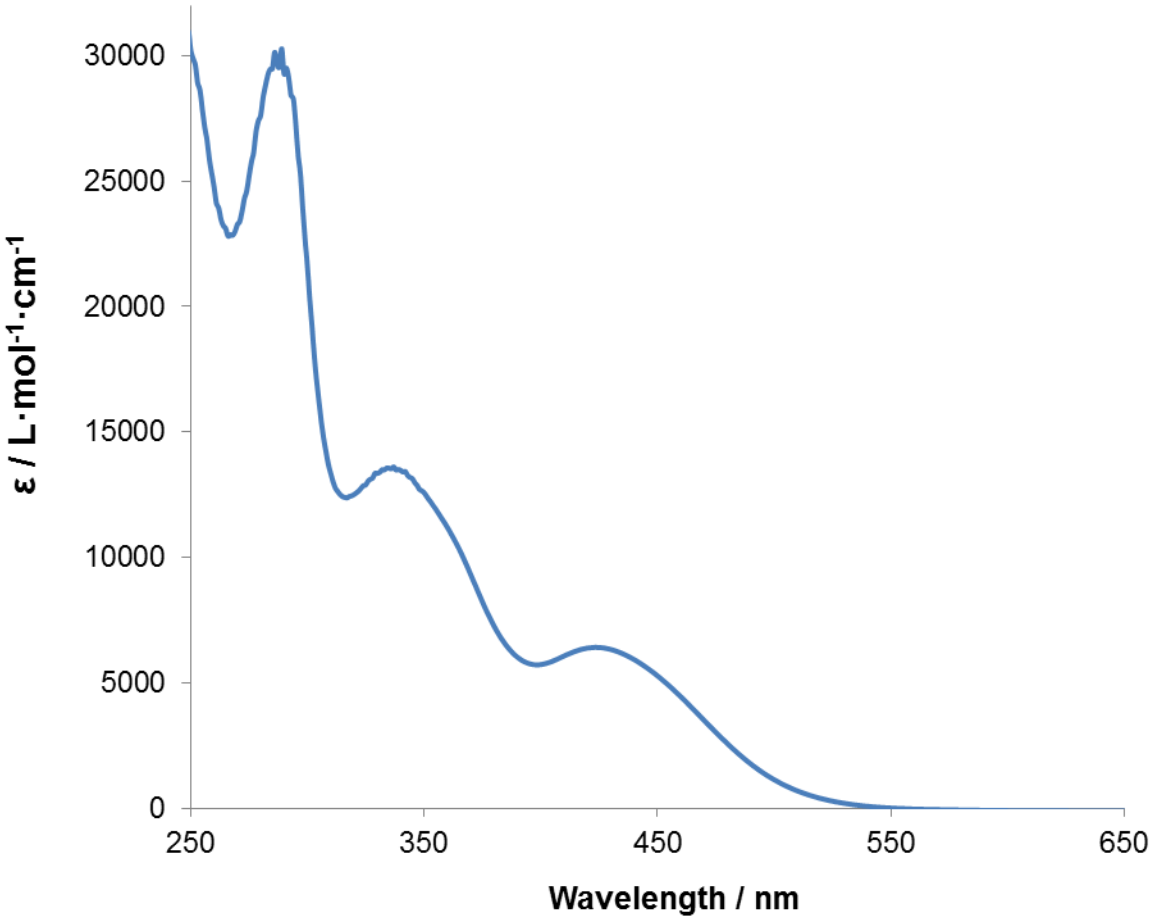

Figure S15. Room temperature UV/vis-NIR absorption spectra for **[K(DME)$_2$]$_2$L^{Ar}** (THF, 0.089 mM).

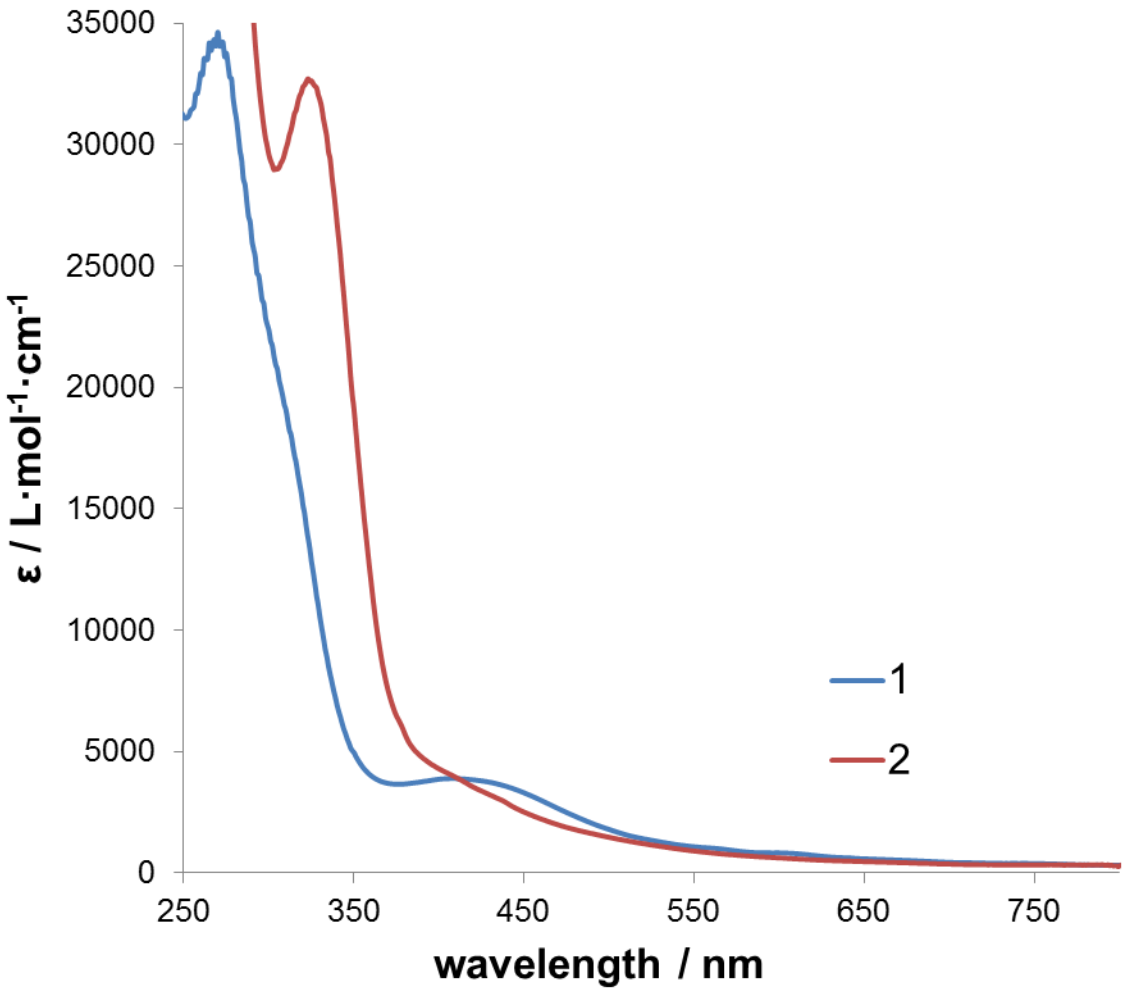

Figure S16. UV-vis absorption spectra for **1**•DME (THF, 0.059 mM) and **2**•0.5DME. (THF, 0.019 mM) .

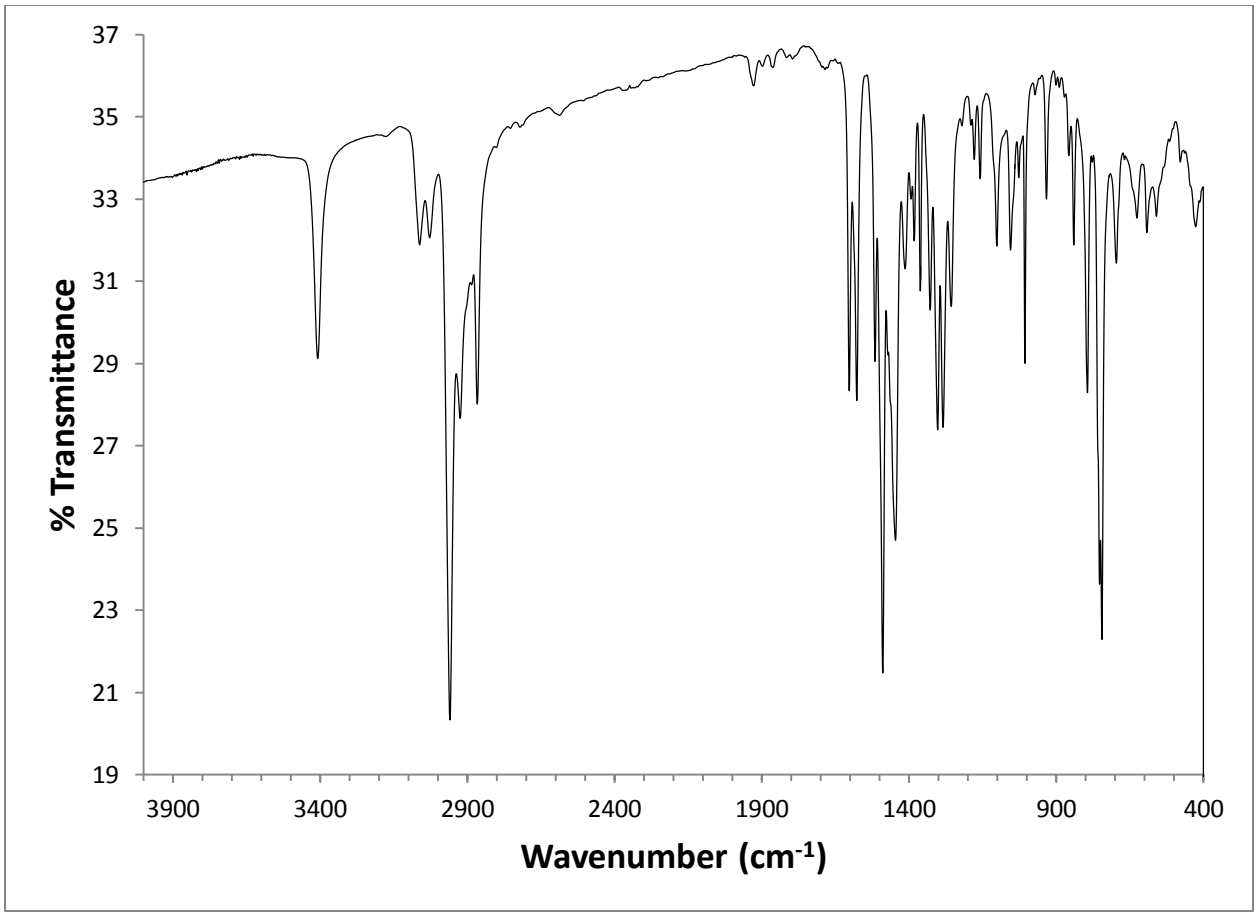

Figure S17. IR spectrum (KBr pellet) of $\mathbf{H_2L^{Ar}}$.

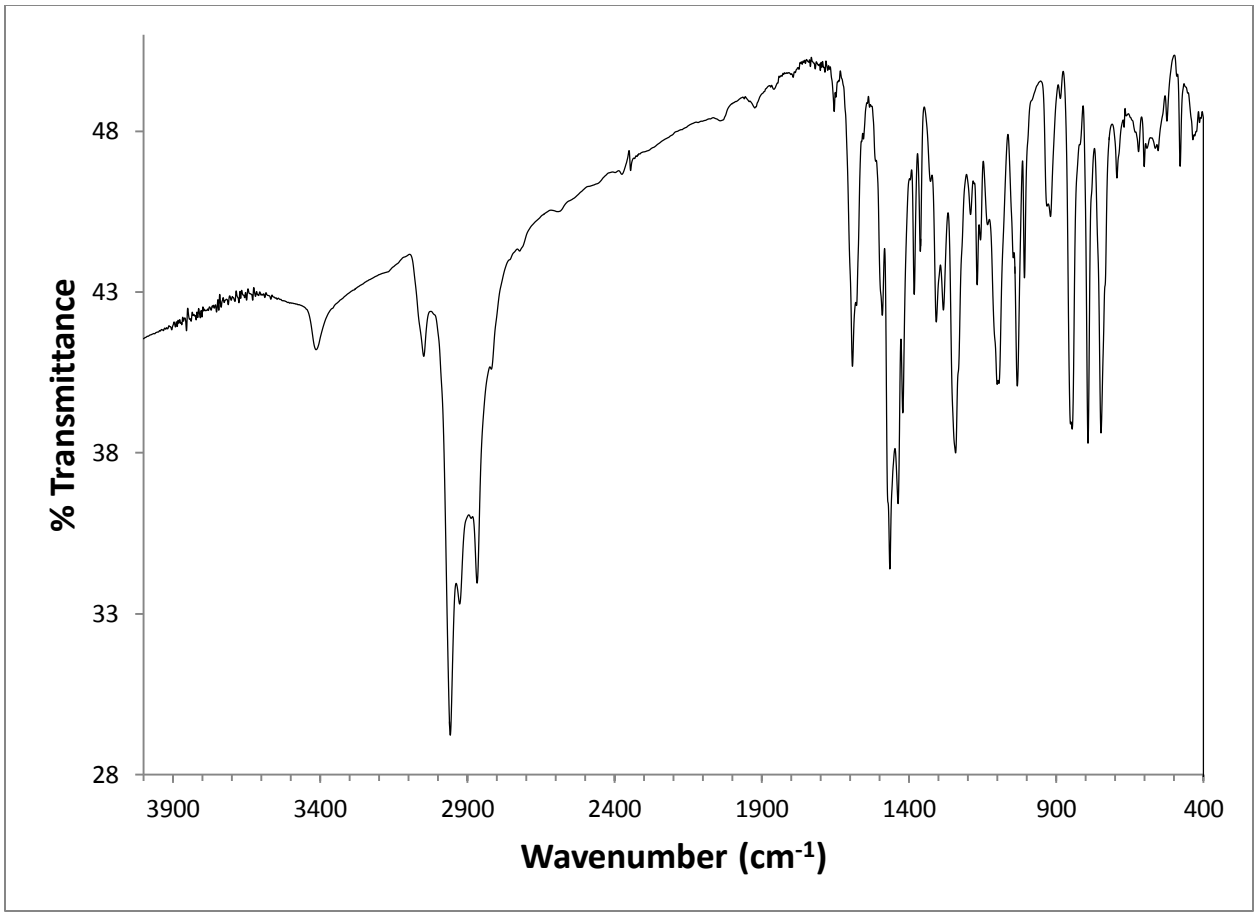

Figure S18. IR spectrum (KBr pellet) of **1**•DME.

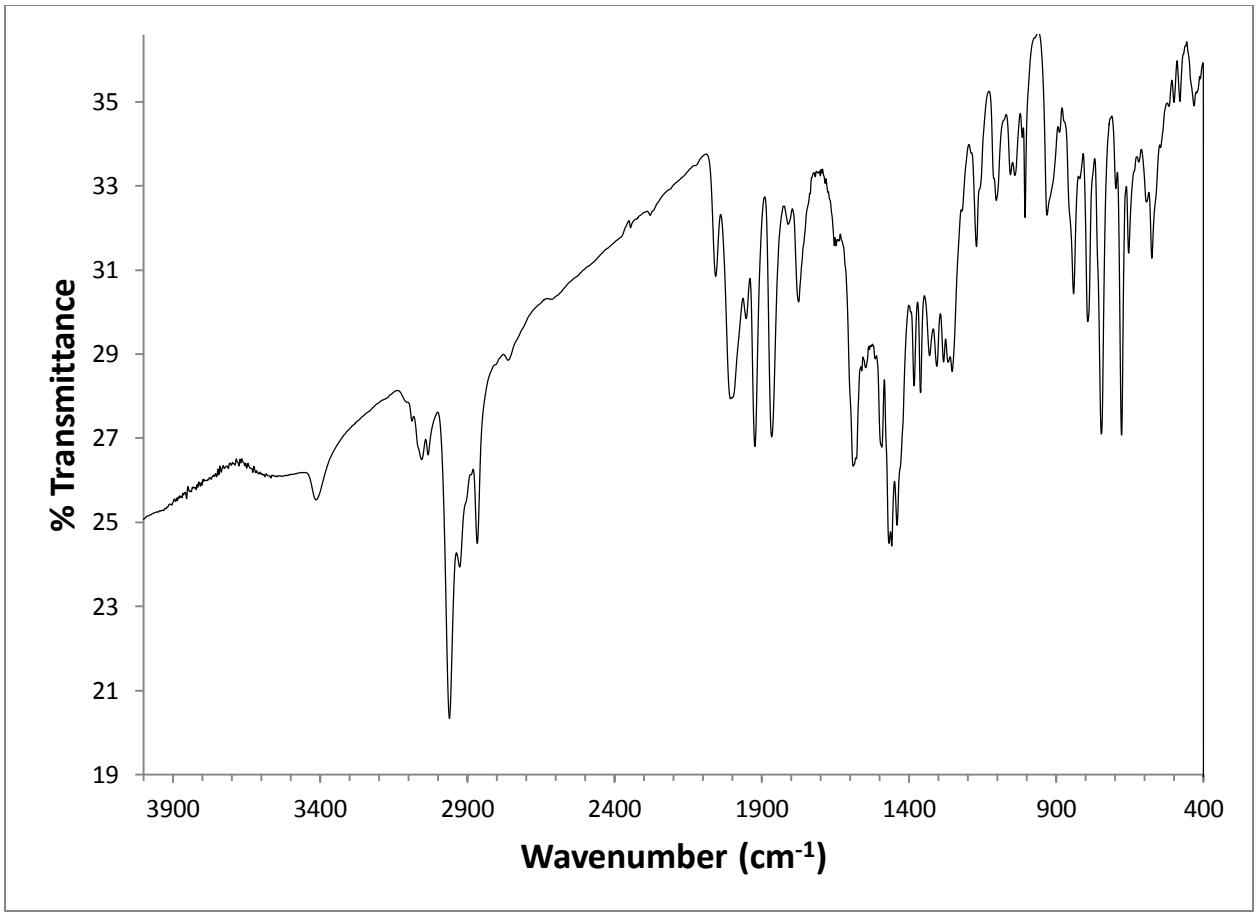

Figure S19. IR spectrum (KBr pellet) of **2**•0.5DME.

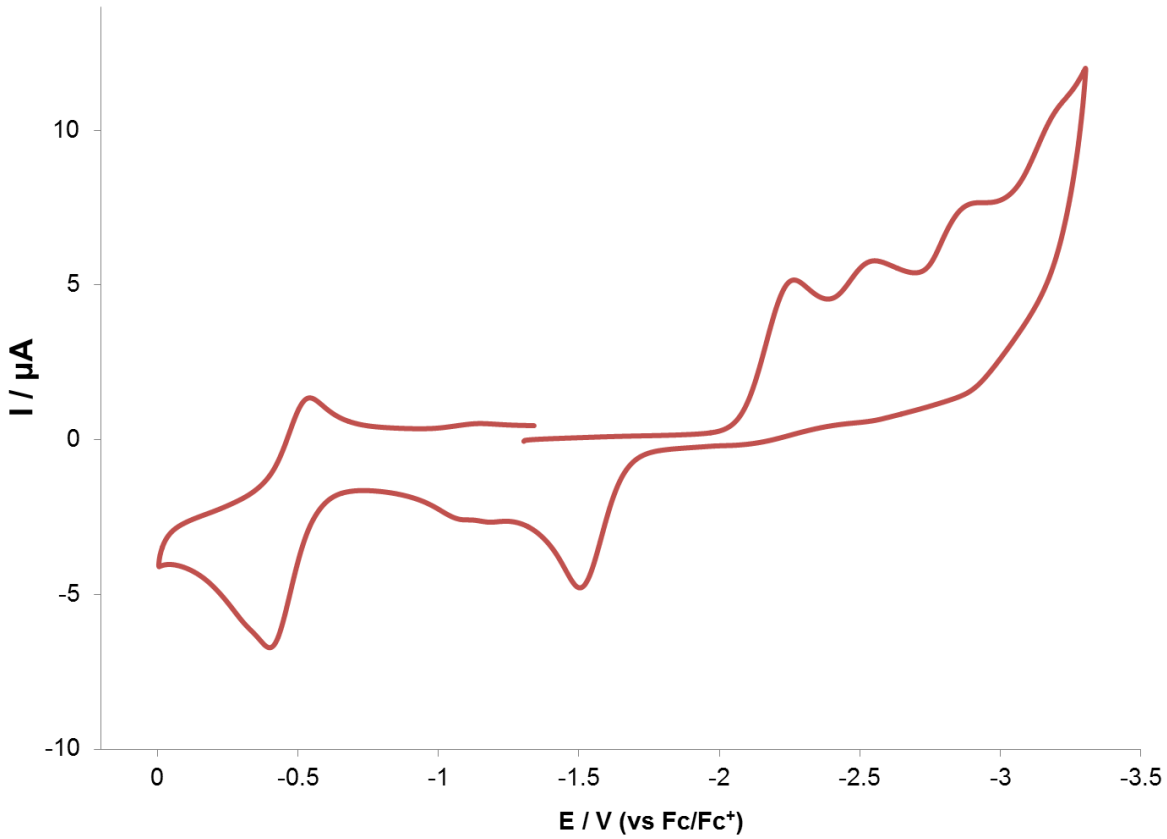

Figure S20. Room temperature cyclic voltammogram of **2**•0.5DME. vs $Fc^{+/0}$ (THF, 0.1 M $[NBu_4][PF_6]$ as supporting electrolyte) at a scan rate of 250 mV/s.

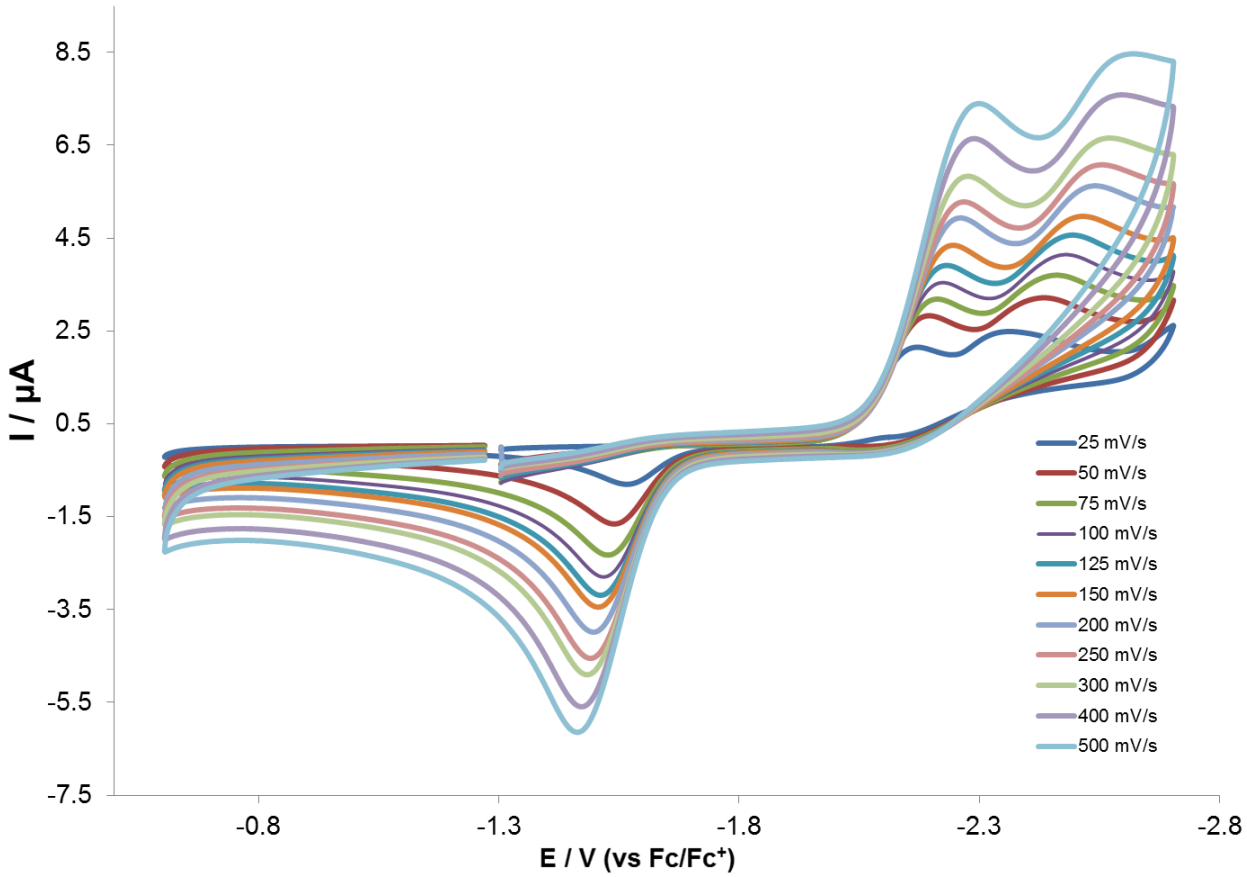

Figure S21. Room temperature cyclic voltammogram of **2**•0.5DME vs $Fc^{+/0}$ (THF, 0.1 M $[NBu_4][PF_6]$ as supporting electrolyte) showing its irreversible reduction features as a function of scan rate.

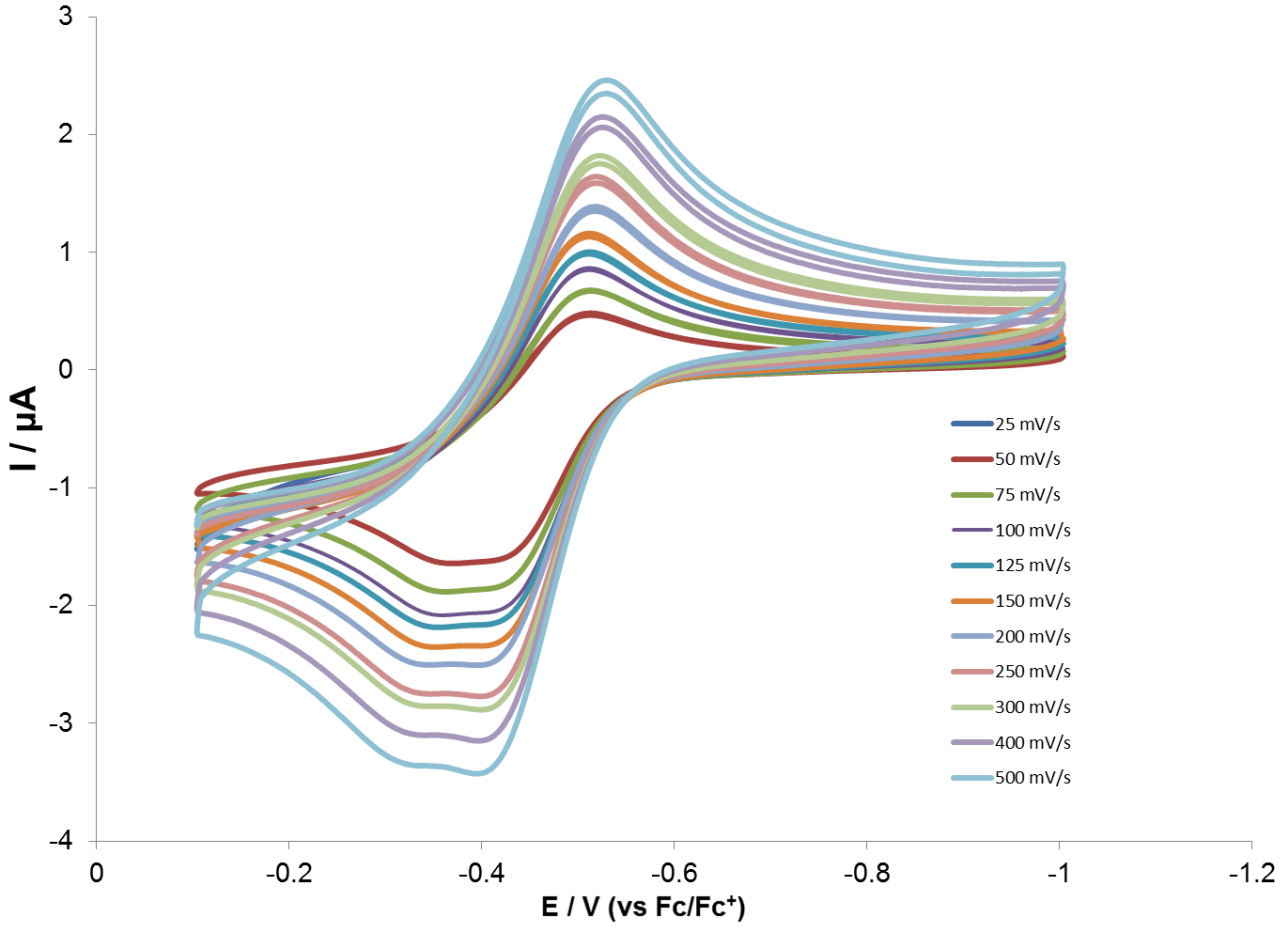

Figure S22. Oxidation feature of **2**•0.5DME vs $Fc^{+/0}$ (THF, 0.1 M $[NBu_4][PF_6]$ as supporting electrolyte) plotted as a function of the scan rate.

Table S1. Select geometric parameters for the RI-PBE optimized geometries of the doublet, quartet, and sextet states of **1**•DME. Distances are in Å and angles in degrees. Average values are reported when noted. Experimental values are included for comparison**.**

Spin	U-N1	U-N2	N1-U1-N2	U-C_{arene} (avg.)	U-$C_{centroid}$	C-C_{arene} (avg.)	U-O (avg.)	U-I
doublet	2.539	2.519	166.8	2.729	2.335	1.413	2.634	3.049
quartet	2.568	2.528	166.3	2.775	2.391	1.411	2.644	3.055
sextet	3.738	2.383	160.2	2.695	2.290	1.421	2.715	3.091
Exp.	2.523(3)	2.558(3)	162.8(1)	2.918	2.562	1.40	2.556	3.1307(3)

Table S2. Select geometric parameters for the RI-PBE optimized geometries of the doublet, quartet, and sextet states of **2**•0.5DME. Distances are in Angstroms and angles in degrees. Average values are reported when noted. Experimental values are included for comparison.

Spin	U-N1	U-N2	N1-U1-N2	U-C_{arene} (avg.)	U-$C_{centroid}$	C-C (arene) (avg.)	U-Fe	Fe-C_{CO} (avg.)	C-O (avg.)	Fe-Ccp (avg.)	C-C (Cp) (avg.)
doublet	2.409	2.332	139.6	2.692	2.291	1.416	2.887	1.741	1.172	2.131	1.429
quartet	2.426	2.344	140.7	2.736	2.343	1.413	2.903	1.742	1.172	2.128	1.431
sextet	2.526	2.411	135.1	2.674	2.268	1.419	2.965	1.763	1.170	2.135	1.430
Exp.	2.354(3)	2.420(2)	137.62(6)	2.82	2.450	1.402	2.9462(3)	1.741	1.163	2.117	1.415

Table S3. Relative RI-PBE energies in kcal/mol for the lowest doublet, quartet, and sextet states of **1**•DME and **2**•0.5DME. The quartet is the ground state and taken as the reference in both cases**.**

Spin	1	2
doublet	9.4	9.4
quartet	0.0	0.0
sextet	36.3	28.3

Table S4. Relative CASPT2 energies in kcal/mol for the lowest doublet, quartet, and sextet states of **2**. The quartet is the ground state and taken as the reference in both cases.

Spin	1	2
doublet		0.1
quartet	0.0	0.0
sextet	97.4	74.3

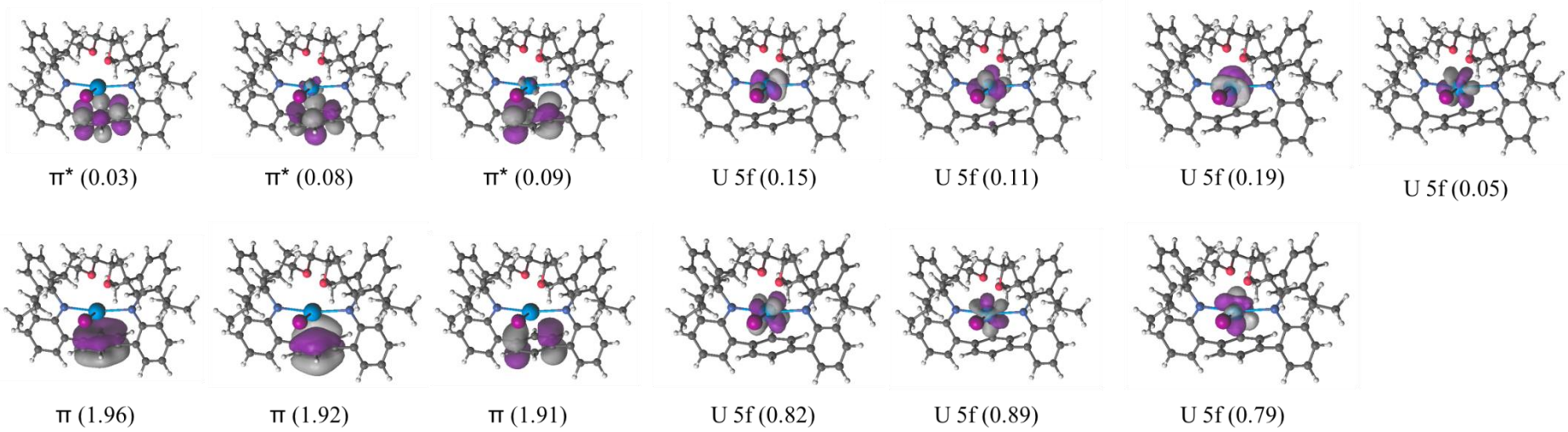

Figure S23. Active natural orbitals for **1**•DME from the (9e, 13o) active space. Occupation numbers are given in parentheses.

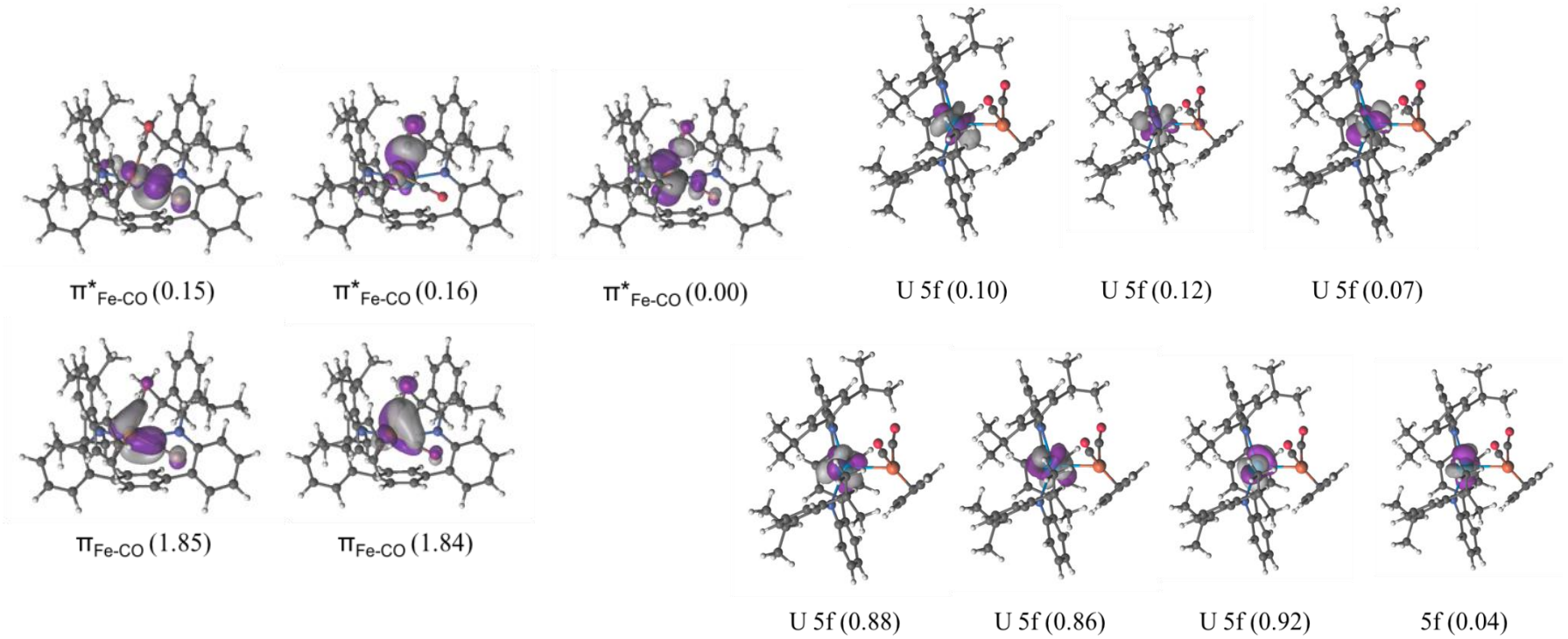

Figure S24. Active natural orbitals for **2**•0.5DME from the (7e, 12o) active space. Occupation numbers are given in parentheses.

Table S5. DFT Optimized Geometries

pbe **1**-doublet
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pbe **1**-quartet

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C	-5.058819	0.596970	0.629201
C	3.035498	-2.615271	0.812397
C	-4.412157	-1.809714	0.431470
C	0.539277	-3.007599	0.742448
C	3.863548	-3.665647	1.207668
C	-0.420431	2.535873	1.000805
C	3.393957	-1.255835	1.007989
C	3.003774	1.060393	0.922400
C	5.099546	-3.415110	1.808353
C	4.668204	-1.030241	1.594061
C	-1.360117	1.562785	1.660246
C	5.491456	-2.086074	1.981842
C	4.049900	3.620623	1.537162
C	-4.383421	-2.128048	1.934544
C	2.816235	1.628927	2.222743
C	-1.171487	-0.524794	2.790725
C	3.329828	2.906417	2.489585
C	2.158501	0.870988	3.376905
C	1.243499	1.748715	4.249786
C	3.201683	0.226526	4.312890

N	-2.152869	-0.783280	-1.304304
N	2.499412	-0.251794	0.612689
O	0.004178	2.014931	-0.269521
O	-0.759941	0.244118	1.650364
I	1.033713	0.144521	-3.482912
U	0.274046	-0.602495	-0.619348
H	3.535008	-4.691933	1.025872
H	5.745647	-4.237301	2.116914
H	6.461787	-1.858817	2.429420
H	5.016429	-0.009526	1.746468
H	0.530388	-3.066215	1.831842
H	-1.611813	-3.214117	0.501376
H	0.651968	-2.943070	-3.160342
H	2.767468	-2.699529	-1.835580
H	-1.647094	-4.983524	-3.073215
H	-3.752860	-4.826220	-4.417809
H	-5.131507	-2.744342	-4.263139
H	-4.434037	-0.880997	-2.821211
H	-5.795676	0.260040	1.362372
H	-5.738302	2.647556	0.696656
H	-4.207611	3.371609	-1.102323
H	-1.520689	3.728623	-3.353504
H	-3.234358	3.914640	-2.957828
H	-2.026171	3.938180	-1.658453
H	-2.841242	0.299056	-3.909752
H	-3.957906	1.685684	-4.027882
H	-2.301999	1.800370	-4.678389
H	-1.383231	1.531171	-2.388993
H	-3.631306	-2.409717	-0.052212
H	-3.388446	-1.985326	2.372123
H	-5.095114	-1.508075	2.499901
H	-4.665653	-3.179044	2.098927
H	-5.900741	-3.352341	0.019544
H	-6.600990	-1.752229	0.359603
H	-5.841860	-2.077989	-1.216979
H	-0.675922	-0.144622	3.696791
H	-2.261751	-0.466260	2.914052
H	-0.875398	-1.563358	2.616707
H	-1.519951	1.883105	2.702326
H	0.475761	2.725112	1.614593
H	1.012690	2.596670	-1.958794
H	0.117478	3.914066	-1.124003
H	1.659932	3.287159	-0.425649
H	-0.954254	3.490412	0.844064
H	-2.333067	1.513855	1.148355
H	1.825719	2.479147	4.830472
H	0.498801	2.311867	3.672447
H	0.709836	1.126249	4.984425
H	3.852074	0.999464	4.751954
H	2.695358	-0.294055	5.140715
H	3.834126	-0.499142	3.791180
H	1.562392	0.061650	2.929677
H	3.446189	0.389909	-1.623800
H	6.336701	1.290262	-1.098017

H	5.634422	-0.271311	-0.610381
H	5.820432	0.120404	-2.335340
H	4.957428	2.933506	-2.459524
H	4.255981	1.681930	-3.498385
H	3.190799	2.757754	-2.581321
H	3.183026	3.344610	3.478979
H	4.444696	4.611220	1.771174
H	4.876167	3.588242	-0.442827

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pbe **1**-singlet

108

FINAL HEAT OF FORMATION = -2819.354110

C	-2.954225	-3.775414	-4.080997
C	-4.087430	-2.976558	-3.861287
C	-3.328344	1.521036	-3.697908
C	-1.816656	-3.608347	-3.287431
C	-4.064834	-2.015536	-2.866387
C	-2.713485	3.402283	-2.156347
C	4.634126	2.039944	-2.580124
C	-2.951886	1.891477	-2.249943
C	-1.753886	-2.653403	-2.265264
C	0.737505	-2.678721	-2.046080
C	-2.903393	-1.796973	-2.057418
C	5.893001	0.273606	-1.316674
C	4.565056	1.050185	-1.410340
C	1.917138	-2.731612	-1.275752
C	-0.544737	-2.586043	-1.432184
C	-3.978801	1.363487	-1.261359
C	1.061118	3.303189	-0.968867
C	-5.027308	2.163846	-0.802938
C	-3.926631	-0.005485	-0.850804
C	-6.014482	1.656170	0.043174
C	-6.197532	-2.746248	-0.052879
C	1.855081	-2.754699	0.146099
C	-0.604167	-2.582144	-0.001206
C	4.210829	1.696284	-0.075314
C	-4.950290	-0.540020	-0.011603
C	4.685393	2.985256	0.205654
C	-5.966611	0.318874	0.425393
C	3.117132	-2.688055	0.918210
C	-4.961765	-1.989055	0.464031
C	0.580643	-2.708036	0.769154
C	3.785693	-3.819497	1.384058
C	-0.370141	2.764871	0.827165
C	3.661814	-1.388089	1.108576
C	3.461499	1.004750	0.923828
C	5.019501	-3.709206	2.034181
C	4.923609	-1.298378	1.740871
C	-1.290119	1.708246	1.376345
C	5.582936	-2.441591	2.193492
C	4.458243	3.595024	1.435980
C	-4.887625	-2.096506	1.996875
C	3.255595	1.615606	2.199479
C	-1.124040	-0.319899	2.603783
C	3.753901	2.906630	2.419973

C	2.580565	0.889648	3.361298
C	1.521716	1.739695	4.082225
C	3.612512	0.417109	4.404774
N	-2.800083	-0.753496	-1.208326
N	2.923858	-0.292927	0.645295
O	0.270270	2.265537	-0.351034
O	-0.524803	0.507959	1.599961
I	1.095573	0.530409	-3.483232
U	0.860735	-0.394756	-0.543523
H	3.335906	-4.801271	1.217749
H	5.538064	-4.599356	2.392082
H	6.556629	-2.335446	2.677260
H	5.389858	-0.320783	1.869398
H	0.526157	-2.779292	1.855979
H	-1.576139	-2.565880	0.490847
H	0.806915	-2.654043	-3.132285
H	2.890637	-2.745594	-1.766720
H	-0.955726	-4.261254	-3.441583
H	-2.960199	-4.533556	-4.865792
H	-4.975082	-3.097410	-4.484639
H	-4.917691	-1.350915	-2.723457
H	-6.744195	-0.075322	1.084133
H	-6.822259	2.300294	0.394854
H	-5.081708	3.206151	-1.121281
H	-1.847210	3.677924	-2.774585
H	-3.574419	3.976885	-2.531855
H	-2.519628	3.731194	-1.124793
H	-3.443584	0.437345	-3.826911
H	-4.275478	2.003912	-3.985712
H	-2.541940	1.855833	-4.390164
H	-1.998173	1.376528	-2.034288
H	-4.073683	-2.491028	0.054555
H	-4.001175	-1.586213	2.399144
H	-5.771255	-1.648175	2.474879
H	-4.840948	-3.151613	2.305168
H	-6.163627	-3.798500	0.266575
H	-7.126064	-2.306467	0.341346
H	-6.253069	-2.727055	-1.149443
H	-1.238442	0.251680	3.539161
H	-2.107772	-0.685655	2.271573
H	-0.451182	-1.164718	2.774142
H	-1.705218	2.065104	2.334635
H	0.399749	3.048321	1.565405
H	1.456818	2.884451	-1.900641
H	0.415225	4.166871	-1.195281
H	1.881206	3.606211	-0.298881
H	-0.962123	3.663856	0.576397
H	-2.127817	1.492456	0.691819
H	1.973684	2.602127	4.594150
H	0.756817	2.121031	3.394704
H	1.018286	1.137801	4.854150
H	4.142881	1.278312	4.839780
H	3.107543	-0.116102	5.225067
H	4.354031	-0.262233	3.968921

H	2.085335	-0.000436	2.944411
H	3.776322	0.317665	-1.646736
H	6.720721	0.954981	-1.064562
H	5.856075	-0.516308	-0.555787
H	6.124640	-0.195962	-2.284897
H	5.509811	2.703034	-2.504437
H	4.723258	1.487764	-3.526187
H	3.732870	2.664014	-2.650873
H	3.601355	3.378338	3.393498
H	4.839495	4.599254	1.631880
H	5.253743	3.520822	-0.556525

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pbe **2**-doublet
106
FINAL HEAT OF FORMATION = -3896.510850

C	-0.328972	-2.124243	-5.508096
C	1.285626	0.321952	-4.828612
C	1.558524	1.684007	-4.761927
C	0.196526	-1.799105	-4.099987
C	-4.103614	-0.659149	-3.881405
C	0.443357	-0.307883	-3.906687
C	1.454678	-2.624961	-3.783805
C	0.962468	2.436560	-3.758806
C	-2.862959	-0.165663	-3.479061
C	-4.711905	-1.715299	-3.196745
C	-0.139002	0.457775	-2.848294
C	0.116941	1.858340	-2.800010
C	-1.722859	3.541178	-2.506890
C	-2.184081	-0.709376	-2.365668
C	-4.046432	-2.287278	-2.109743
C	3.349044	0.360504	-1.597672
C	-0.561890	2.800553	-1.815531
C	-2.795215	-1.815813	-1.696418
C	0.402487	3.814276	-1.184789
C	-0.726740	-2.887852	-0.767976
C	-2.055645	-2.396752	-0.554892
C	2.866603	-0.245017	-0.276862
C	3.820305	-1.379290	0.145482
C	-3.824369	2.024914	0.201485
C	-4.158517	0.646027	0.328560
C	0.118444	-3.137489	0.311977
C	3.397325	1.981594	0.803431
C	2.698020	0.768158	0.856301
C	-2.549321	-2.379828	0.777172
C	-4.095162	2.680790	1.454307
C	-4.606219	0.448039	1.672910
C	3.402906	2.856786	1.885126
C	-0.325026	-2.940139	1.648417
C	-1.267741	2.252553	1.706110
C	-1.693848	-2.636314	1.865885
C	-4.583724	1.711202	2.360109
C	1.941822	0.456042	2.028269
C	0.700504	-2.980637	2.714423
C	2.717952	2.517592	3.046873
C	1.519843	-1.824732	2.790997

C	1.979991	1.333374	3.154170
C	-2.135025	0.250147	3.129963
C	2.659468	-1.876828	3.617277
C	0.961649	-4.093380	3.511029
C	2.913866	-3.001070	4.403986
C	2.058931	-4.104483	4.379427
C	1.296755	1.037532	4.487616
C	0.287679	2.122187	4.904764
C	2.330982	0.886273	5.621914
H	0.414296	-1.897741	-6.286644
H	-1.240739	-1.552669	-5.730940
H	-0.572000	-3.194776	-5.584189
H	1.738133	-0.274743	-5.623694
H	2.218067	2.155611	-5.492510
H	-4.605628	-0.202730	-4.737003
H	2.275555	-2.376346	-4.473471
H	-2.409813	0.667583	-4.017673
H	1.250172	-3.702242	-3.884386
H	1.147671	3.510939	-3.719661
H	-5.682958	-2.097702	-3.512818
H	-0.592779	-2.100101	-3.402089
H	-1.346470	4.149090	-3.343998
H	-2.470156	2.843593	-2.910485
H	1.814062	-2.439093	-2.760689
H	3.326777	-0.402603	-2.387243
H	2.727372	1.201078	-1.930995
H	-2.225312	4.222908	-1.802843
H	-4.489036	-3.133241	-1.578638
H	4.389760	0.708091	-1.514110
H	0.815035	4.499914	-1.939344
H	-0.363698	-3.030644	-1.782209
H	-1.002135	2.191841	-1.006636
H	3.922323	-2.117403	-0.665127
H	-3.451486	2.506112	-0.696867
H	-4.145147	-0.090653	-0.468908
H	1.887209	-0.735550	-0.485906
H	1.242138	3.321664	-0.675997
H	-0.122965	4.425151	-0.439320
H	3.963051	2.239024	-0.091730
H	4.818923	-0.964858	0.351005
H	1.148718	-3.455294	0.141062
H	3.477858	-1.899716	1.048162
H	-3.584476	-2.095337	0.959997
H	3.952698	3.797918	1.825769
H	-3.926698	3.732381	1.669732
H	-4.937005	-0.491860	2.107607
H	-4.862673	1.878502	3.396379
H	-2.062881	-2.543443	2.886464
H	3.346038	-1.030726	3.635542
H	2.745612	3.199688	3.899211
H	0.311898	-4.968025	3.431811
H	-0.520553	2.249306	4.177838
H	0.752671	0.087769	4.392885
H	3.796833	-3.010838	5.046676

H	0.781052	3.097519	5.031460
H	2.257684	-4.975180	5.005178
H	3.091732	0.128474	5.400683
H	2.847159	1.840036	5.811820
H	-0.166570	1.849335	5.868734
H	1.823584	0.592348	6.552683
N	-0.976966	-0.180842	-1.870309
N	1.140910	-0.729140	2.004289
O	-0.459829	3.101406	1.737991
O	-1.934811	-0.300812	4.144223
Fe	-2.619079	1.157724	1.723430
U	-0.617559	-0.516475	0.487695

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pbe **2**-quartet

106

FINAL HEAT OF FORMATION = -3896.525690

C	-0.327527	-2.132301	-5.523623
C	1.273664	0.328784	-4.852096
C	1.544366	1.691565	-4.785058
C	0.195058	-1.796396	-4.117065
C	-4.107391	-0.702873	-3.890868
C	0.432920	-0.302603	-3.930129
C	1.458197	-2.612866	-3.795864
C	0.948344	2.442308	-3.780486
C	-2.873225	-0.193484	-3.490591
C	-4.703682	-1.765044	-3.204738
C	-0.152971	0.461751	-2.872150
C	0.103646	1.862070	-2.822176
C	-1.731493	3.548476	-2.522785
C	-2.182058	-0.725410	-2.377411
C	-4.030812	-2.323693	-2.115728
C	3.345204	0.364752	-1.591629
C	-0.573579	2.801338	-1.833640
C	-2.785243	-1.836239	-1.705639
C	0.393293	3.807900	-1.195232
C	-0.722198	-2.885218	-0.757371
C	-2.045035	-2.407036	-0.557882
C	2.875007	-0.245518	-0.268490
C	3.835656	-1.376191	0.147837
C	-3.829666	2.069769	0.211123
C	-4.151089	0.685609	0.313520
C	0.125321	-3.119590	0.327307
C	3.401259	1.981126	0.814023
C	2.708009	0.764079	0.868275
C	-2.534672	-2.351202	0.772696
C	-4.119312	2.703988	1.470876
C	-4.611743	0.463336	1.649972
C	3.409245	2.853671	1.897687
C	-0.330716	-2.944798	1.662759
C	-1.284818	2.288976	1.721592
C	-1.687030	-2.623518	1.869812
C	-4.607735	1.715977	2.356707
C	1.959325	0.444665	2.043738
C	0.692690	-2.987784	2.731474
C	2.729190	2.510108	3.061129

C	1.521635	-1.836384	2.803874
C	1.996822	1.322572	3.169576
C	-2.149664	0.276008	3.132461
C	2.659796	-1.900333	3.632500
C	0.942051	-4.100752	3.531230
C	2.903181	-3.024603	4.422092
C	2.038133	-4.120249	4.400742
C	1.315503	1.023807	4.503004
C	0.307209	2.108052	4.922484
C	2.351480	0.869174	5.635162
H	0.414478	-1.903749	-6.302799
H	-1.243281	-1.568317	-5.749484
H	-0.562718	-3.204924	-5.595116
H	1.728207	-0.267021	-5.646799
H	2.202694	2.164596	-5.515775
H	-4.615227	-0.253526	-4.746904
H	2.277710	-2.363640	-4.486895
H	-2.431107	0.644125	-4.031716
H	1.260366	-3.692091	-3.889590
H	1.132861	3.516867	-3.740107
H	-5.670437	-2.159500	-3.518728
H	-0.592680	-2.099598	-3.417947
H	-1.352635	4.155594	-3.359327
H	-2.481827	2.854317	-2.926806
H	1.817007	-2.418059	-2.774115
H	3.322098	-0.397177	-2.382400
H	2.715862	1.201817	-1.919914
H	-2.230706	4.231858	-1.817985
H	-4.463681	-3.171770	-1.579864
H	4.384173	0.719101	-1.515180
H	0.812664	4.493857	-1.945731
H	-0.346983	-3.011182	-1.770007
H	-1.017869	2.189818	-1.028273
H	3.934742	-2.115027	-0.662530
H	-3.451240	2.568109	-0.675504
H	-4.121856	-0.039278	-0.494607
H	1.897463	-0.741972	-0.471285
H	1.229098	3.309387	-0.685551
H	-0.131369	4.418628	-0.449074
H	3.960802	2.242956	-0.083782
H	4.834229	-0.958287	0.346340
H	1.159879	-3.424740	0.161556
H	3.500447	-1.896385	1.053599
H	-3.564960	-2.047126	0.948885
H	3.954923	3.797133	1.837764
H	-3.963244	3.753683	1.703825
H	-4.939519	-0.485545	2.067088
H	-4.899321	1.864653	3.392312
H	-2.059756	-2.518001	2.888072
H	3.353994	-1.060318	3.649699
H	2.755745	3.191798	3.913821
H	0.284410	-4.969625	3.453418
H	-0.499022	2.238809	4.193922
H	0.770401	0.074724	4.406147

H	3.785879	-3.040736	5.065074
H	0.801396	3.082341	5.053993
H	2.227772	-4.990978	5.029106
H	3.113139	0.113583	5.409272
H	2.866645	1.822954	5.827918
H	-0.149601	1.832204	5.884393
H	1.846379	0.570537	6.565681
N	-0.982033	-0.179730	-1.891308
N	1.157134	-0.738335	2.018722
O	-0.476001	3.137340	1.759254
O	-1.950644	-0.282275	4.143605
Fe	-2.634135	1.191133	1.731477
U	-0.595293	-0.458787	0.487162

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pbe **2**-singlet

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FINAL HEAT OF FORMATION = -3896.467820

C	-0.376786	-2.187392	-5.602483
C	1.252026	0.275396	-4.959168
C	1.552064	1.631409	-4.876725
C	0.168386	-1.846358	-4.206301
C	-4.142130	-0.629915	-3.815521
C	0.419040	-0.354300	-4.028727
C	1.435647	-2.662282	-3.898369
C	1.001009	2.379663	-3.842844
C	-2.855295	-0.207970	-3.496351
C	-4.781287	-1.613610	-3.051309
C	-0.125701	0.408516	-2.948010
C	0.169677	1.800700	-2.875153
C	-1.660851	3.470268	-2.458530
C	-2.152342	-0.735866	-2.380697
C	-4.093289	-2.191611	-1.980662
C	3.423130	0.449307	-1.529014
C	-0.466080	2.719098	-1.842069
C	-2.796438	-1.791464	-1.638314
C	0.523841	3.714454	-1.223842
C	-0.731930	-2.900347	-0.765391
C	-2.052790	-2.426319	-0.528082
C	2.992619	-0.193718	-0.207120
C	3.985440	-1.310437	0.170573
C	-4.088353	2.126804	0.195544
C	-4.435148	0.749862	0.304454
C	0.150408	-3.127168	0.300376
C	3.541222	1.993144	0.944933
C	2.822490	0.790714	0.948406
C	-2.526877	-2.408180	0.819450
C	-4.272131	2.743297	1.484396
C	-4.797397	0.506448	1.663948
C	3.513712	2.856256	2.036926
C	-0.278541	-2.953095	1.648876
C	-1.454268	2.333415	1.604399
C	-1.643637	-2.666229	1.897194
C	-4.710568	1.746342	2.390347
C	2.024568	0.468215	2.088860
C	0.771247	-2.981249	2.694821

C	2.768528	2.516296	3.160926
C	1.587388	-1.813962	2.787773
C	2.017099	1.336552	3.221198
C	-2.253750	0.289007	3.027775
C	2.737531	-1.879365	3.610558
C	1.061210	-4.108351	3.457809
C	3.009404	-3.015808	4.367980
C	2.166024	-4.129146	4.318818
C	1.252559	1.034321	4.507483
C	0.252502	2.143231	4.878614
C	2.209248	0.822706	5.697380
H	0.352009	-1.960660	-6.394636
H	-1.296902	-1.625388	-5.816089
H	-0.611456	-3.260504	-5.666678
H	1.679320	-0.316970	-5.771402
H	2.200919	2.102441	-5.617100
H	-4.658772	-0.175049	-4.663125
H	2.242133	-2.423280	-4.608038
H	-2.381229	0.579867	-4.083299
H	1.232591	-3.741799	-3.973497
H	1.212387	3.448683	-3.789552
H	-5.791468	-1.941640	-3.299013
H	-0.606855	-2.145100	-3.490821
H	-1.326030	4.104189	-3.294025
H	-2.418949	2.776372	-2.848126
H	1.812169	-2.454187	-2.886001
H	3.380960	-0.294883	-2.336756
H	2.778512	1.288587	-1.820451
H	-2.134626	4.126744	-1.712188
H	-4.557801	-2.995554	-1.404780
H	4.461157	0.811909	-1.479124
H	0.918058	4.410475	-1.978493
H	-0.376604	-3.007543	-1.787175
H	-0.873261	2.086425	-1.031075
H	4.084960	-2.032091	-0.654953
H	-3.759233	2.630281	-0.708314
H	-4.428633	0.021721	-0.502358
H	2.018790	-0.699095	-0.382761
H	1.376306	3.206810	-0.751816
H	0.027581	4.316013	-0.451620
H	4.145765	2.253576	0.075795
H	4.979265	-0.877840	0.362667
H	1.183813	-3.418956	0.107761
H	3.674572	-1.856760	1.070195
H	-3.557223	-2.117410	1.021341
H	4.080059	3.789091	2.013372
H	-4.084387	3.786785	1.722291
H	-5.110709	-0.446151	2.083046
H	-4.926763	1.884253	3.445824
H	-1.994569	-2.583104	2.925375
H	3.412703	-1.024440	3.646725
H	2.761606	3.189981	4.020429
H	0.422015	-4.989029	3.362711
H	-0.470643	2.338723	4.080059

H	0.685152	0.105037	4.357218
H	3.896022	-3.032108	5.005472
H	0.770297	3.089347	5.097953
H	2.377430	-5.012829	4.921903
H	2.931609	0.018573	5.514037
H	2.772120	1.742945	5.917595
H	-0.306645	1.852883	5.780296
H	1.634542	0.560358	6.598253
N	-0.934788	-0.216929	-1.956648
N	1.214225	-0.706804	2.039611
O	-0.675345	3.202771	1.682362
O	-2.091034	-0.206695	4.075687
Fe	-2.796001	1.206188	1.622683
U	-0.661550	-0.539516	0.534113