Supporting Information for
Exploring the Interaction of Pyridine-Based Chalcones with Trinuclear Silver(I) Pyrazolate Complex

Arina Olbrykh[1,2], Aleksei Titov[1], Alexander Smol'yakov[1,3], Oleg Filippov[1], Elena S. Shubina[1]*

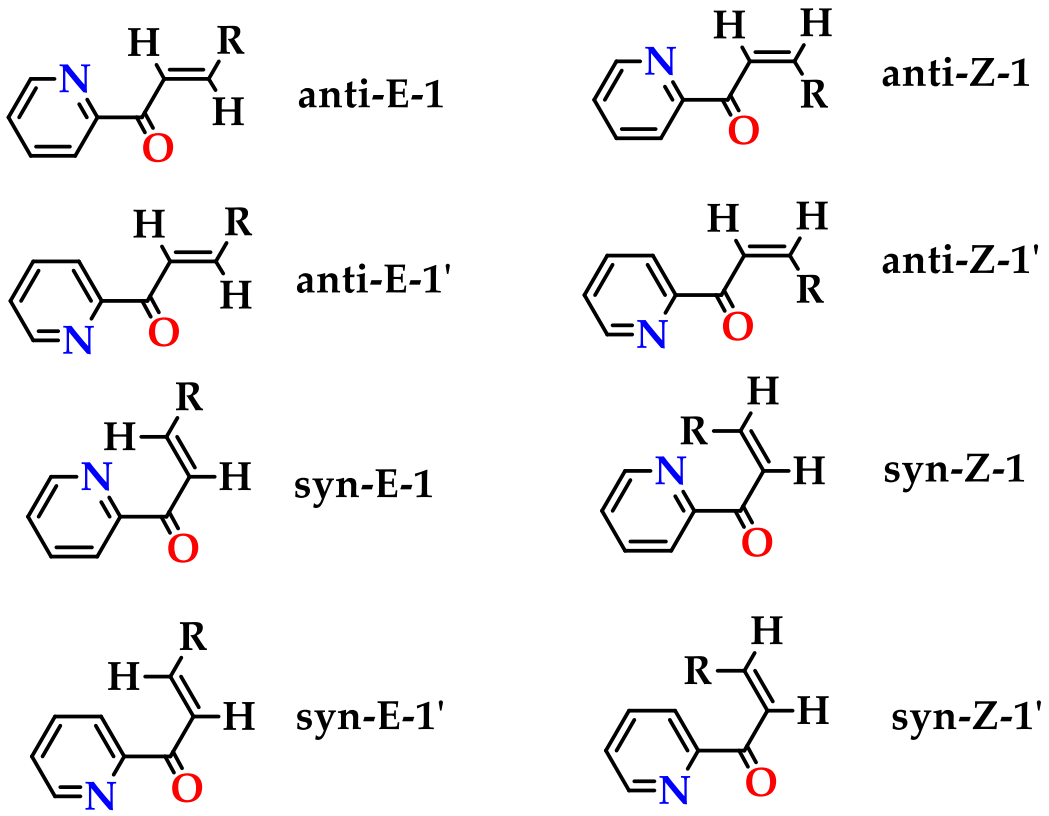
1 A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Vavilov Str., 28,

119991 Moscow, Russia; arinaolbr@gmail.com (A.O.); tit@ineos.ac.ru (A.T.); rengenhik@gmail.com (A.S.), h-bond@ineos.ac.ru (O.F.); shu@ineos.ac.ru (E.S.S.)

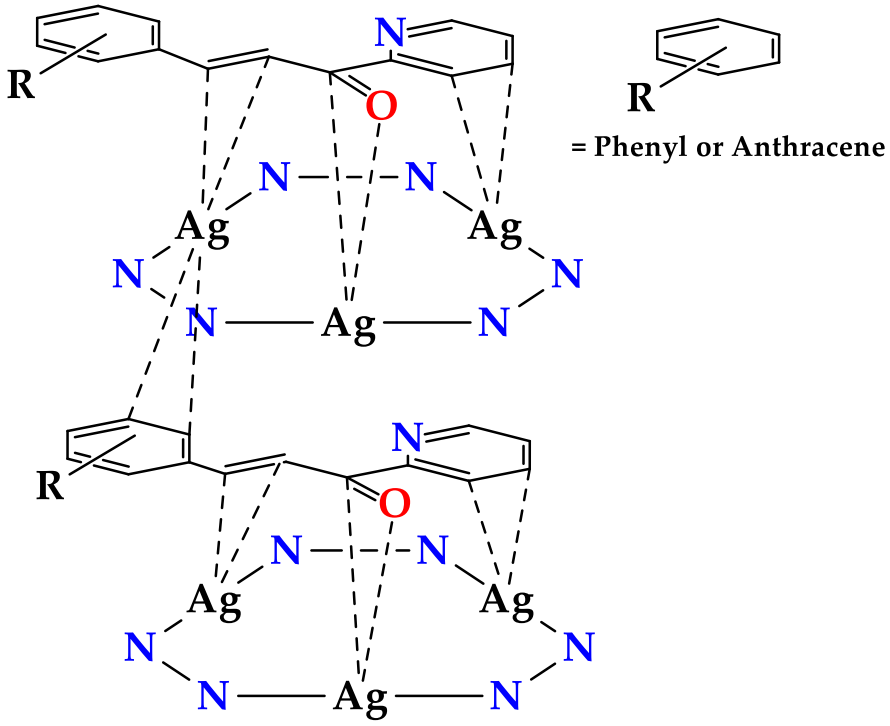
2 Higher Chemical College, Mendeleev University of Chemical Technology of Russia, Miusskaya Sq. 9, 125047 Moscow, Russia; arinaolbr@gmail.com (A.O.);

3 Plekhanov Russian University of Economics, Stremyanny per. 36, Moscow 117997, Russia; rengenhik@gmail.com (A.S.)

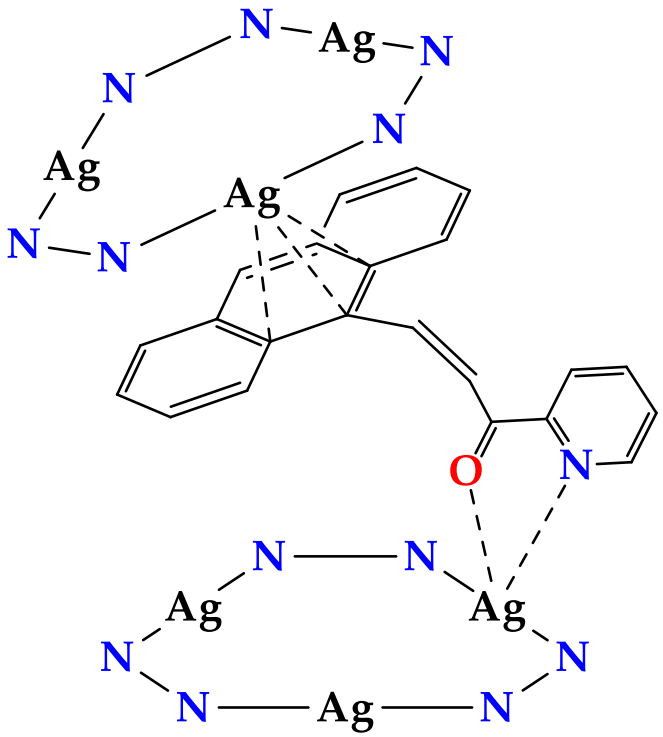
* Correspondence shu@ineos.ac.ru (E.S.S.)



Scheme S1. Possible isomers for pyridine- based chalcones.



Scheme S2. Schematic representation of supramolecular packing of E-**1Ag** and E-**2Ag**.



Scheme S3. Schematic representation of supramolecular packing of Z-**1Ag**.

Table S1. Crystal data, data collection, and structure refinement parameters for E-**1Ag** and E-**2Ag**, Z-**1Ag**.

Complex	E-**1Ag**	E-**2Ag**	Z-**1Ag**
Empirical formula	$C_{37}H_{18}Ag_3F_{18}N_7O$	$C_{29}H_{14.5}Ag_3F_{18}N_7O1.25$	C37H18Ag3F18N7O
Formula weight	1242.19	1146.59	1242.19
Temperature/K	100	100	100
Crystal system	triclinic	monoclinic	monoclinic
Space group	P1	P21/c	P21/n
a/Å	7.8326(2)	12.8452(5)	13.1222(8)
b/Å	11.0556(2)	22.8123(8)	14.3897(10)
c/Å	12.8446(3)	13.0509(5)	20.6671(14)
α/°	114.7540(10)	90	90
β/°	102.7180(10)	115.750(2)	91.486(3)
γ/°	94.9140(10)	90	90
Volume/Å^3	965.22(4)	3444.5(2)	3901.1(4)
Z	1	4	4
ϱ_{calc}g/cm^3	2.137	2.211	2.115
μ/mm^{-1}	1.638	1.826	1.621
F(000)	600	2202	2400
Crystal size/mm^3	0.24 × 0.17 × 0.08	0.24 × 0.17 × 0.11	0.21 × 0.15 × 0.11
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.102 to 51.996	3.898 to 59.302	3.72 to 51.996
Reflections collected	9600	47024	44445
Independent reflections	5359 [R_{int} = 0.0170, R_{sigma} = 0.0306]	9692 [R_{int} = 0.0512, R_{sigma} = 0.0415]	7611 [R_{int} = 0.0415, R_{sigma} = 0.0295]
Data/restraints/parameters	5359/3/595	9692/66/584	7611/6/604
Goodness-of-fit on F^2	1.037	1.032	1.151
Final R indexes [I>=2σ (I)]	R_1 = 0.0153, wR_2 = 0.0367	R_1 = 0.0388, wR_2 = 0.0888	R_1 = 0.0424, wR_2 = 0.0955
Final R indexes [all data]	R_1 = 0.0155, wR_2 = 0.0368	R_1 = 0.0512, wR_2 = 0.0956	R_1 = 0.0462, wR_2 = 0.0978
Largest diff. peak /hole / e Å^{-3}	0.44/-0.34	1.77/-0.99	1.55/-0.9

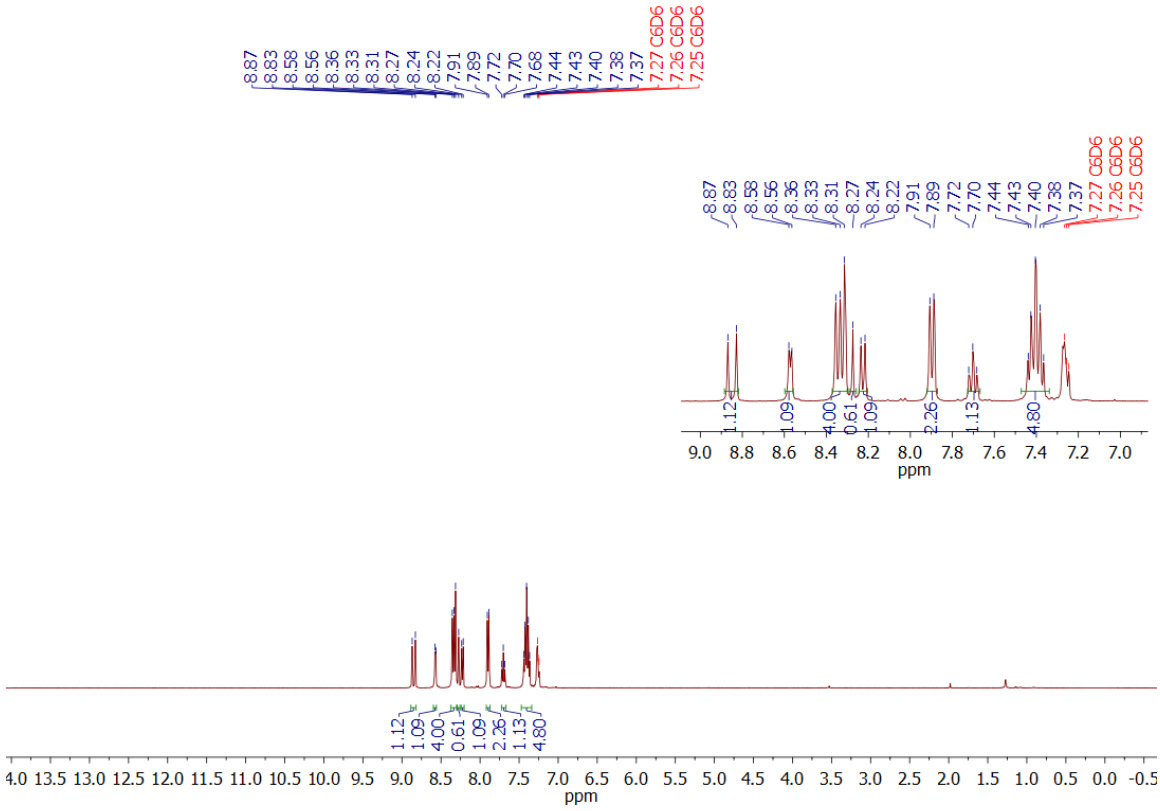


Figure S1. ^{1}H NMR spectrum of E-**1** in the mixture CCl_4/benzene-d_6 (9/1).

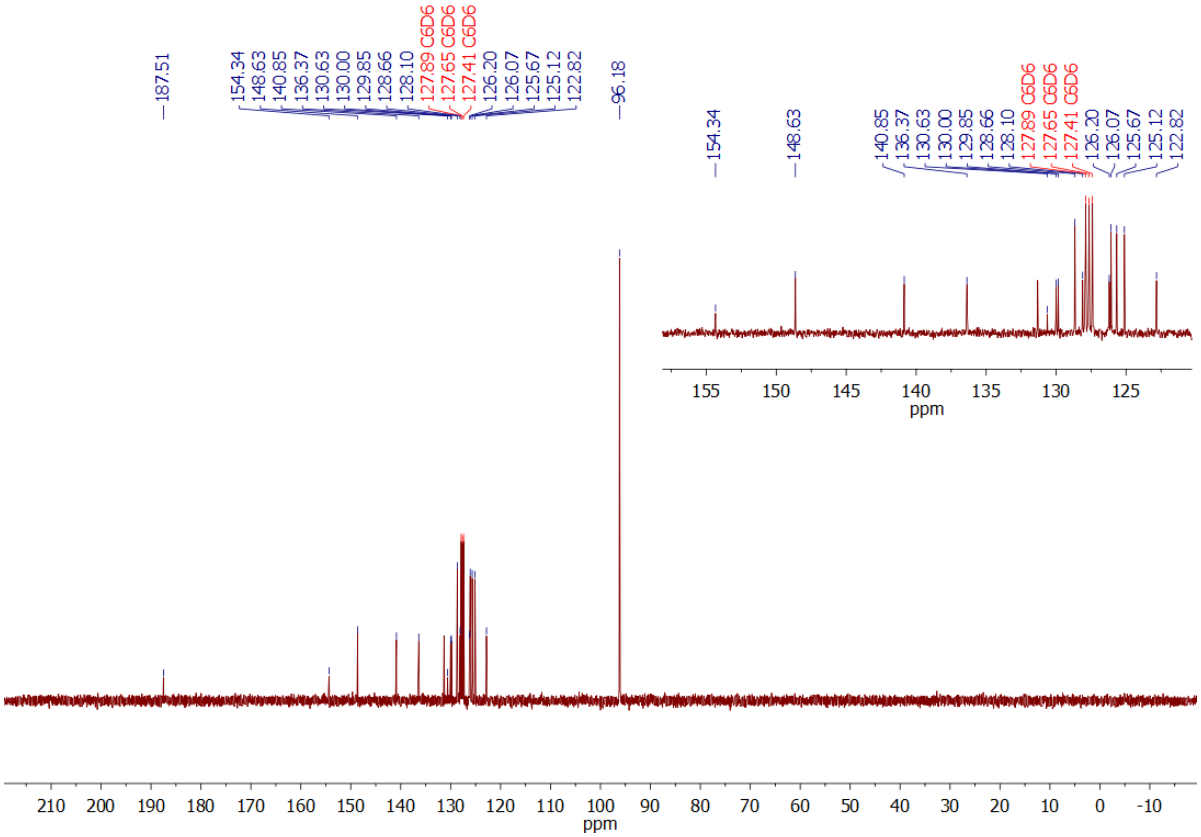


Figure S2. ^{13}C NMR spectrum of E-**1** in CCl_4/benzene-d_6 (9/1) mixture.

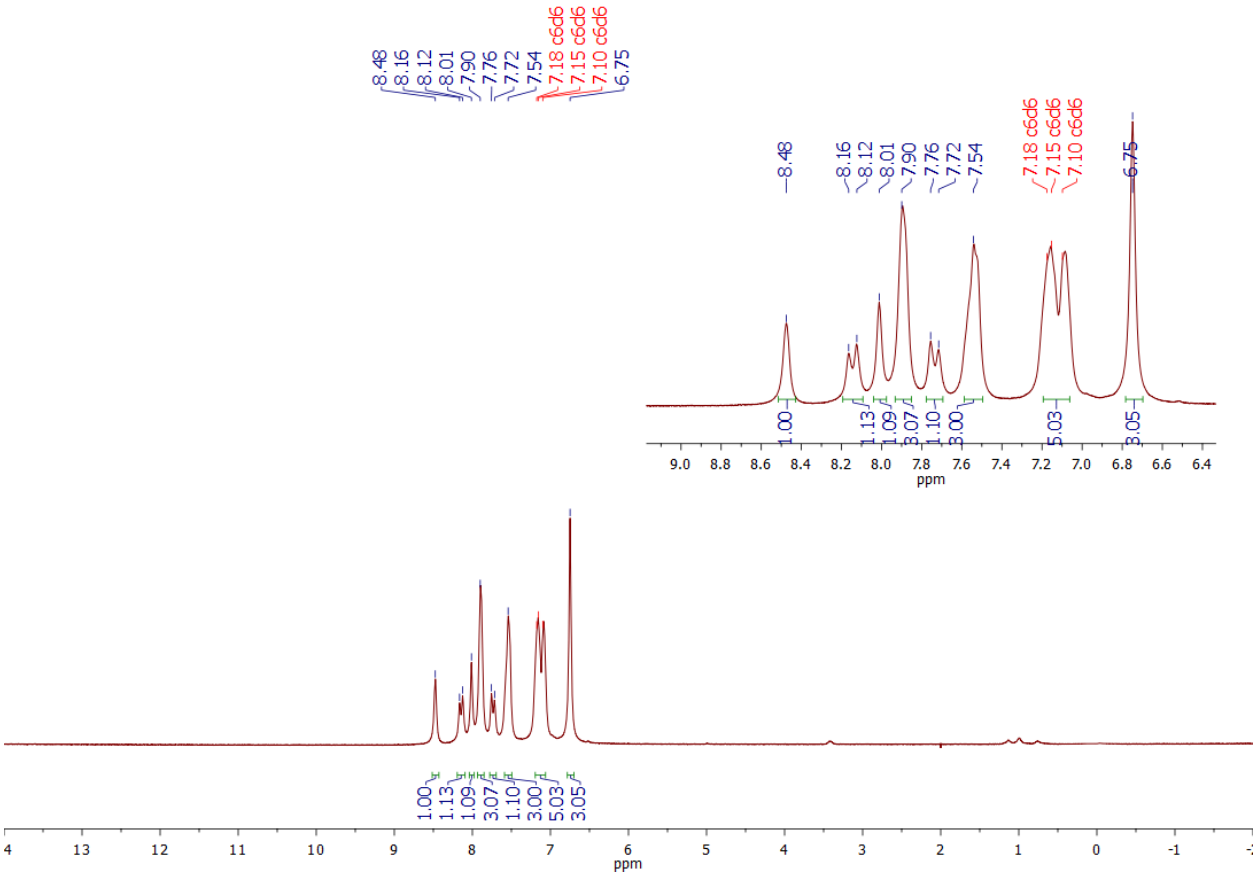


Figure S3. ^{1}H NMR spectrum of E-**1** +1 eq. $[AgPz]_3$ in CCl_4/benzene-d_6 (9/1) mixture.

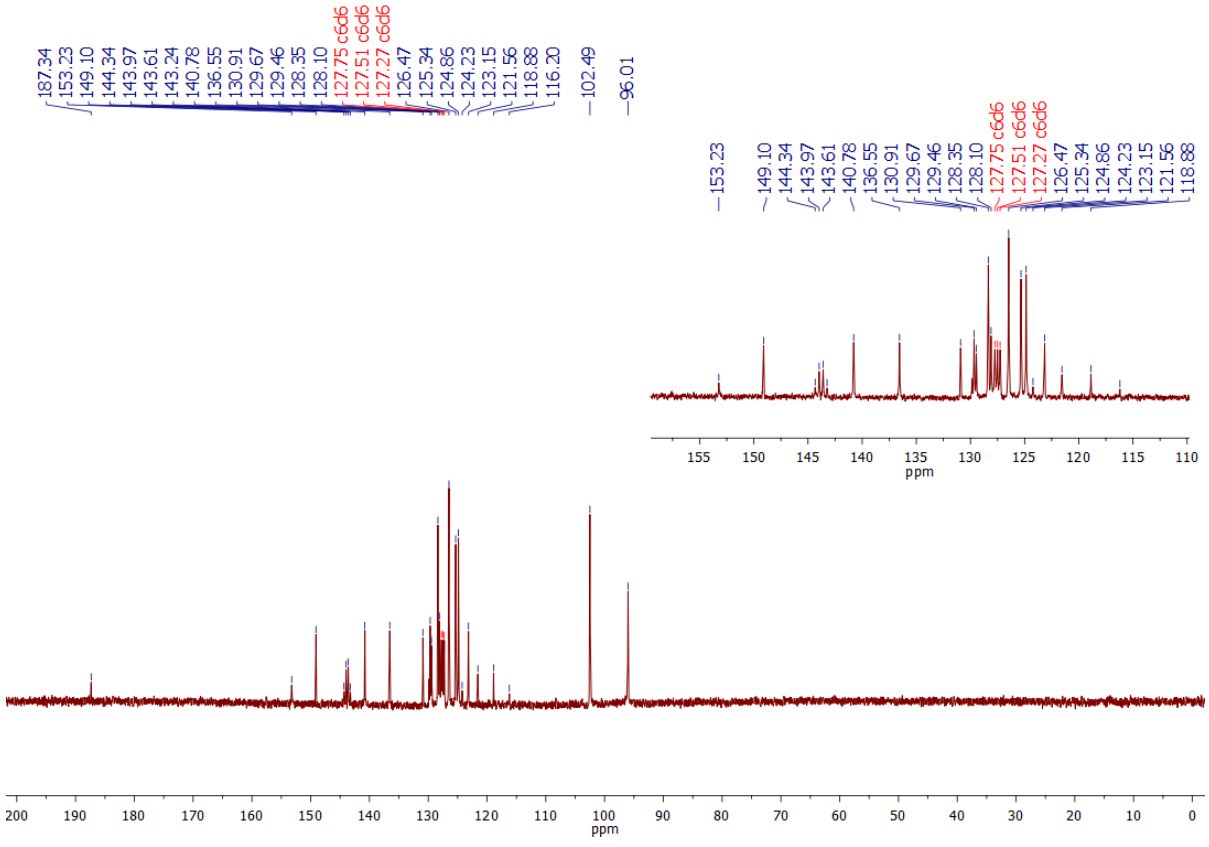


Figure S4. ^{13}C NMR spectrum of E-**1** + 1 eq. $[AgPz]_3$ in CCl_4/benzene-d_6 (9/1) mixture.

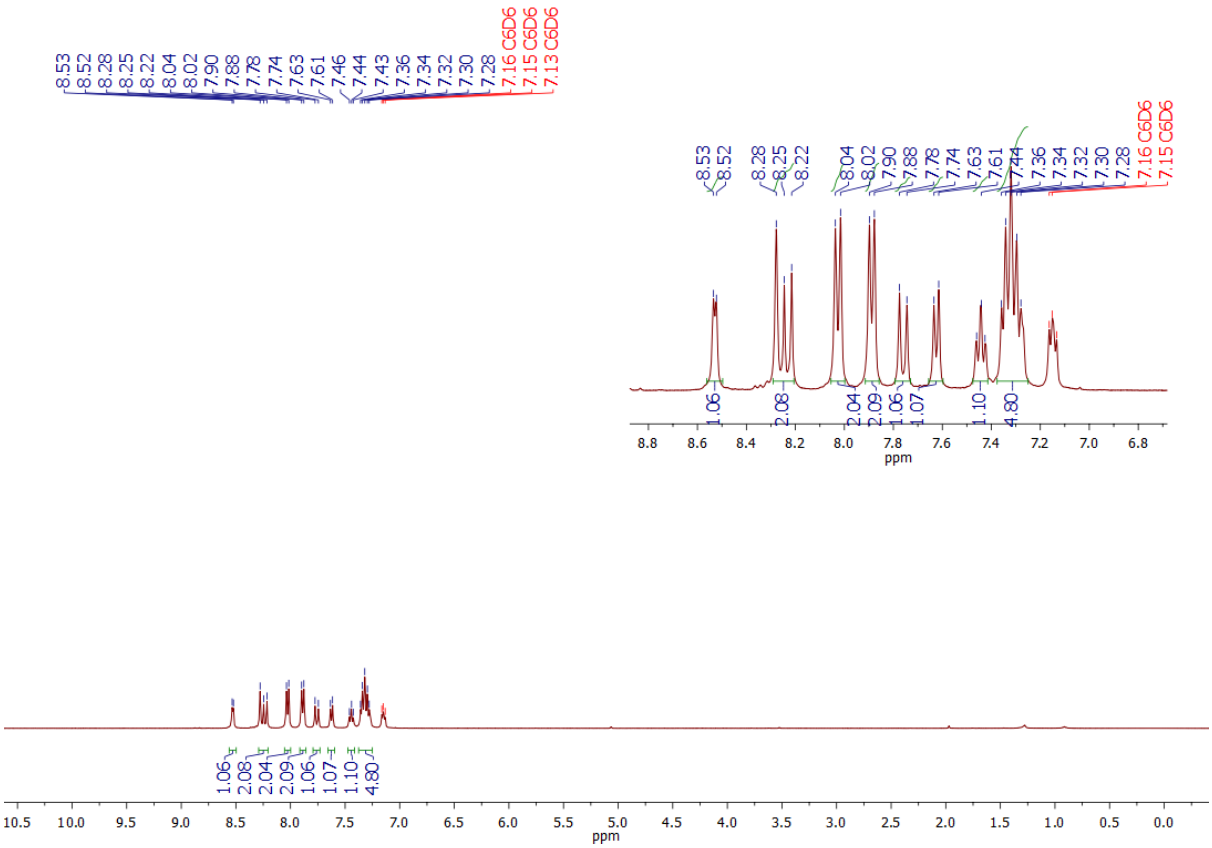


Figure S5. ^{1}H NMR spectrum of Z-**1** in CCl_4/benzene-d_6 (9/1) mixture.

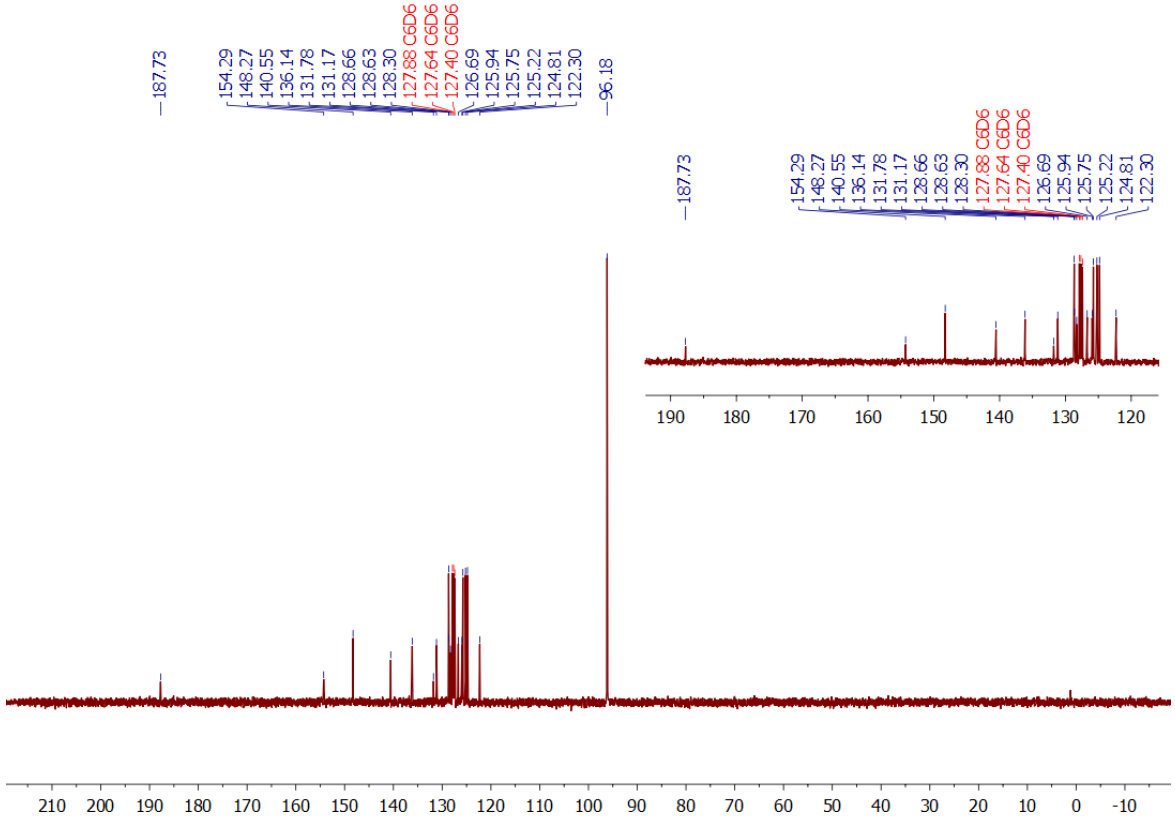


Figure S6. ^{13}C NMR spectrum of Z-**1** in CCl_4/benzene-d_6 (9/1) mixture.

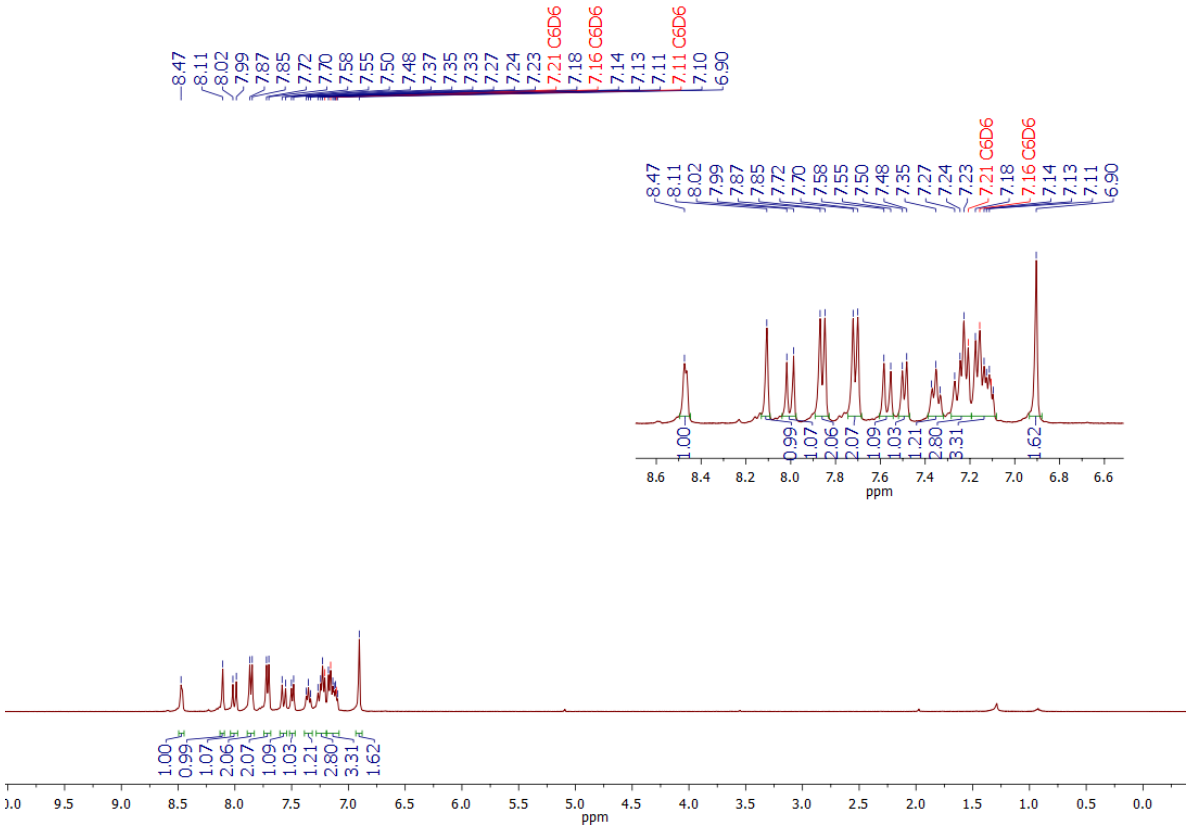


Figure S7. ^{1}H NMR spectrum of Z-**1**+0.5 eq. [AgPz]$_3$ in CCl_4/benzene-d_6 (9/1) mixture.

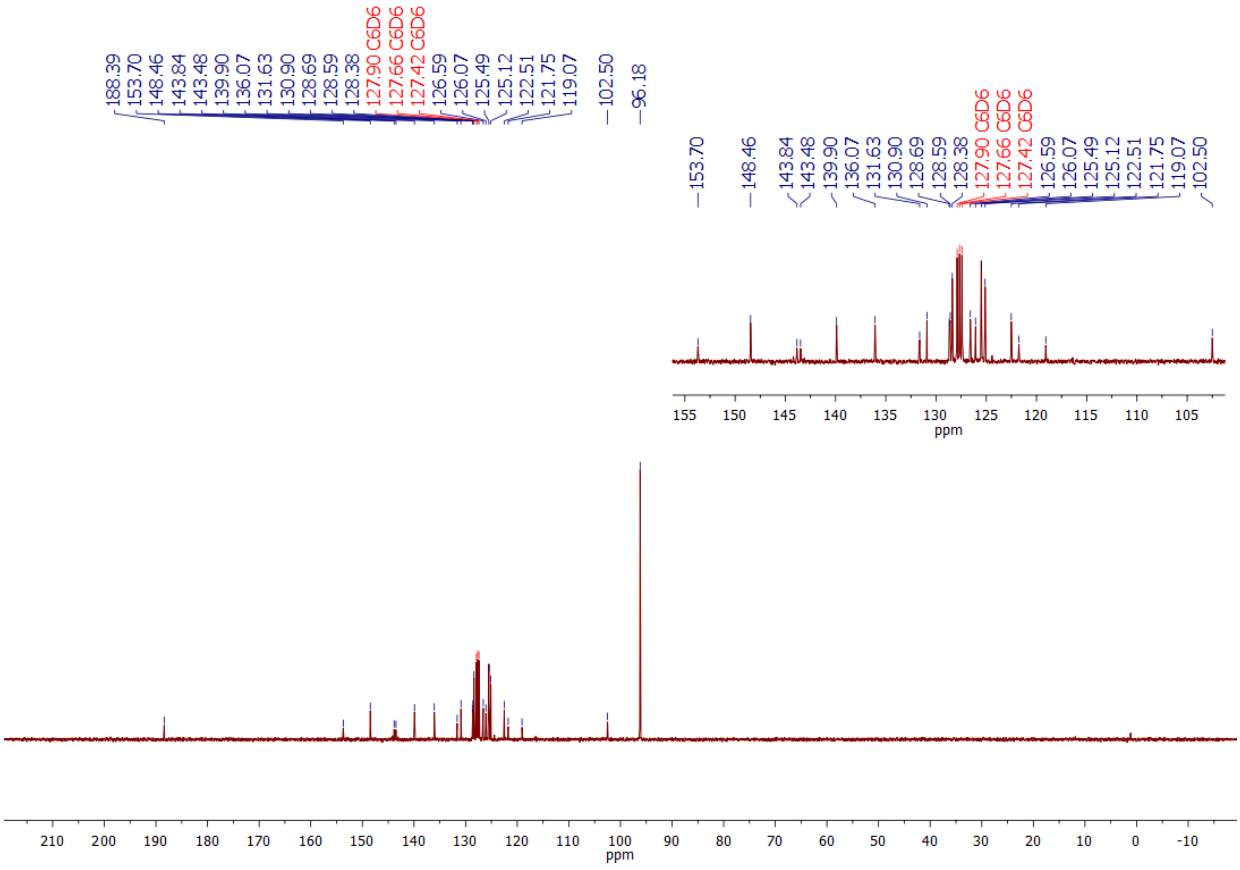


Figure S8. ^{13}C NMR spectrum of Z-**1**+0.5 eq. [AgPz]$_3$ in CCl_4/benzene-d_6 (9/1) mixture.

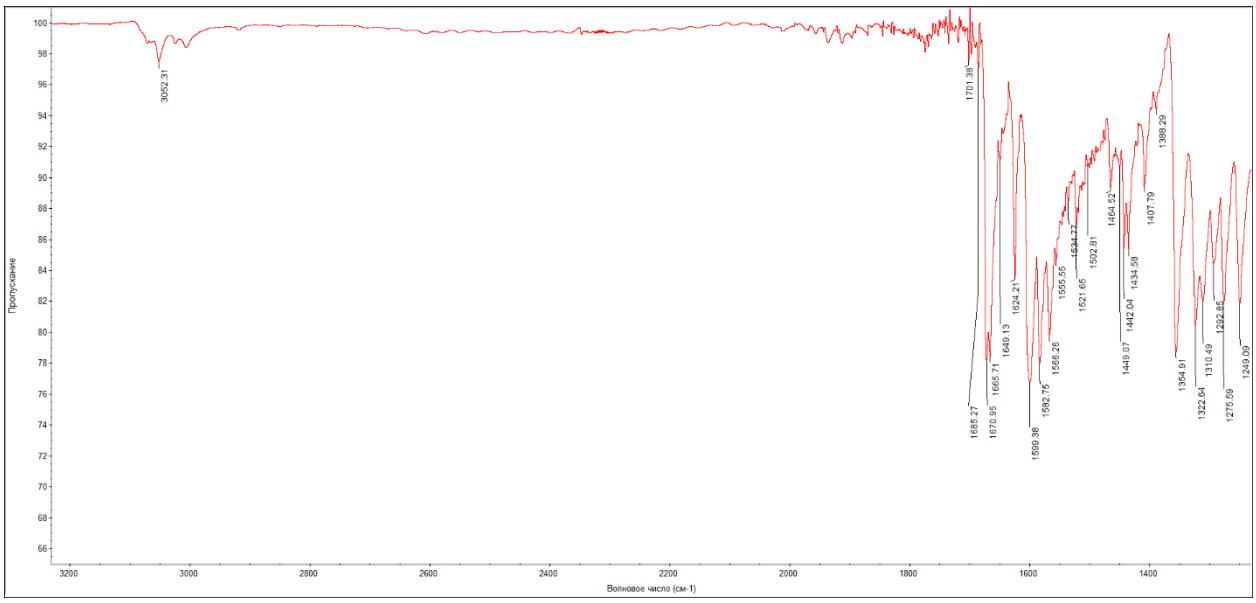


Figure S9. IR spectra of E-**1** in KBr.

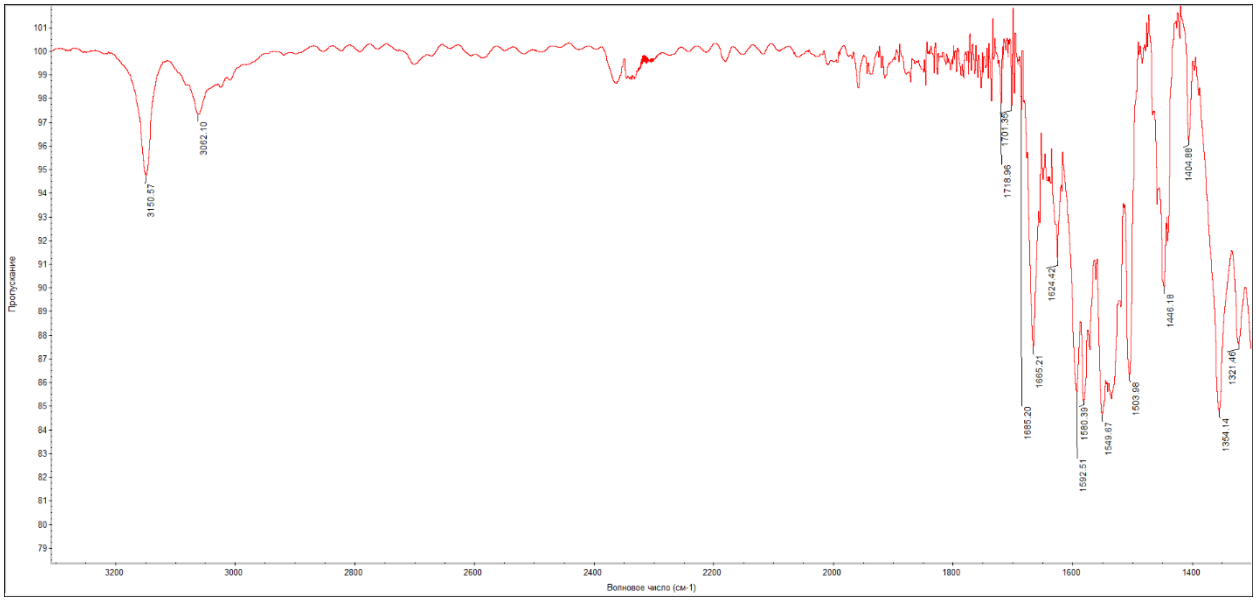


Figure S10. IR spectra of E-**1Ag** in KBr.

Figure S11. IR spectra of Z-**1** in KBr.

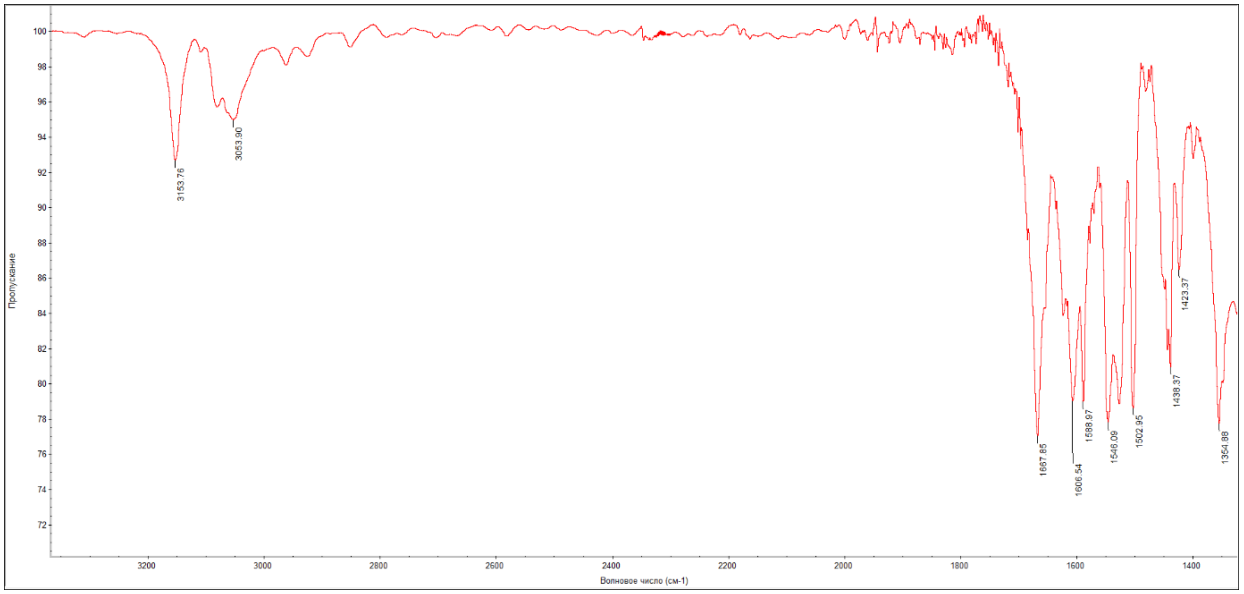


Figure S12. IR spectra of Z-**1Ag** in KBr.

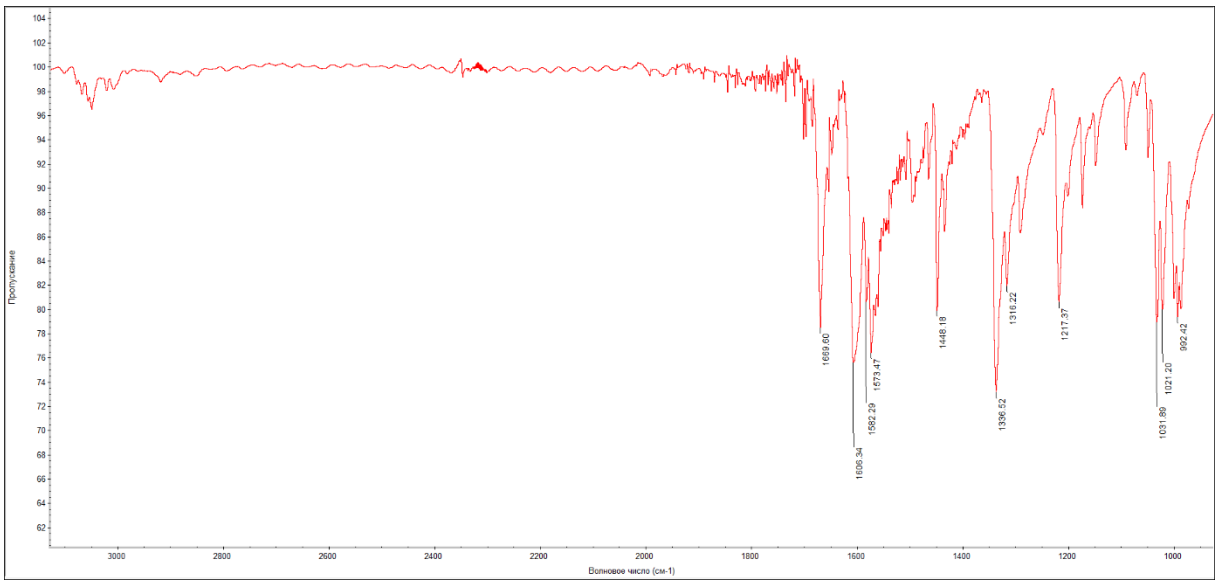


Figure S13. IR spectra of E-**2** in KBr.

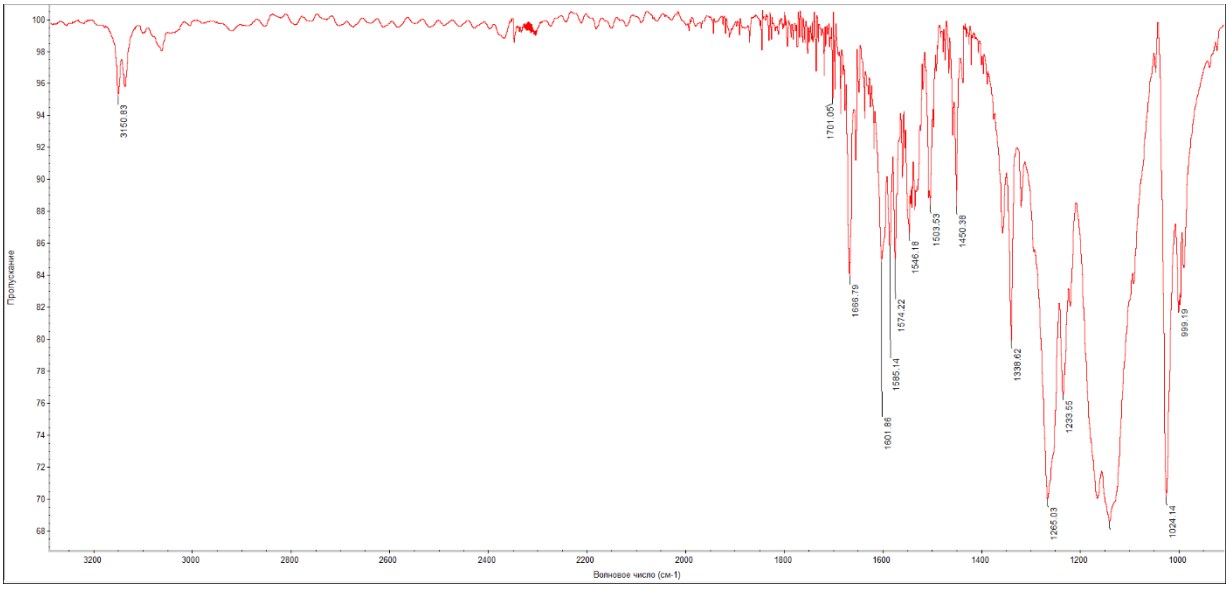


Figure S14. IR spectra of E-**2Ag** in KBr.

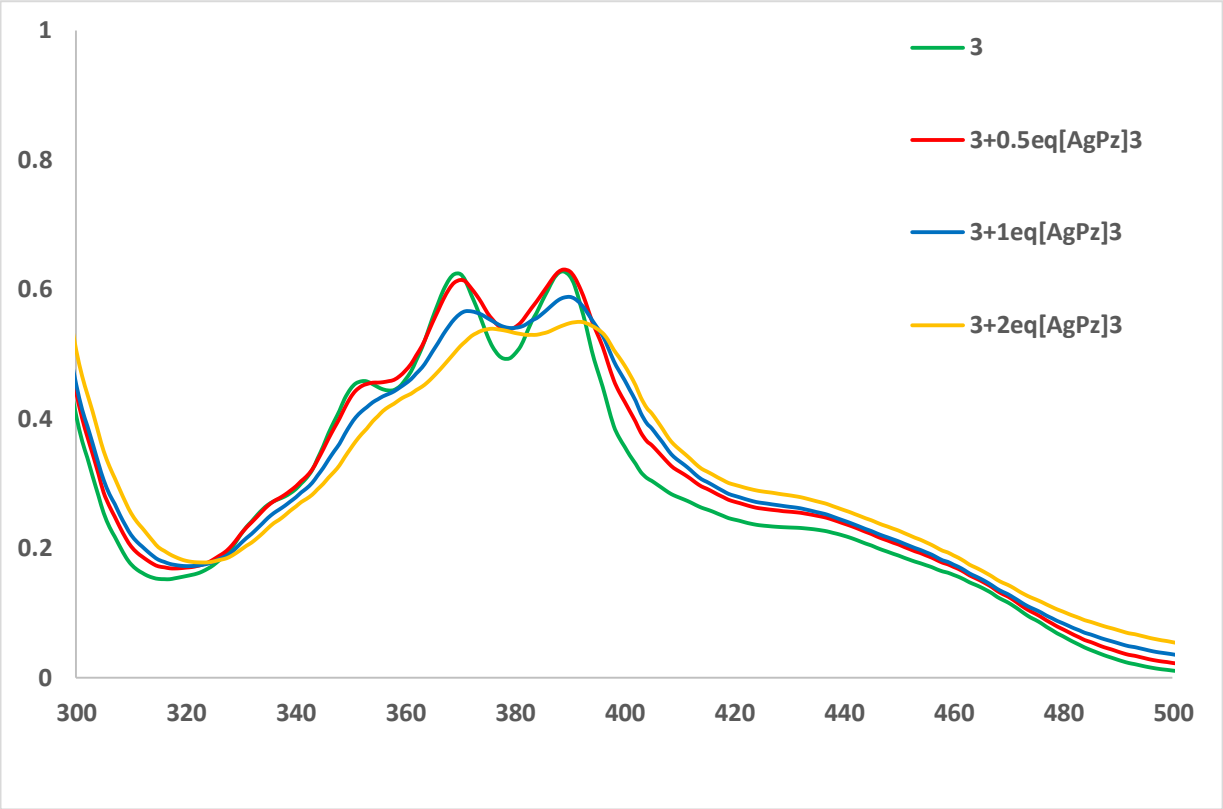


Figure S15. UV-vis spectra of Z-**1** + $[AgPz]_3$ c=0.015M d=0.0047 cm in CCl_4.

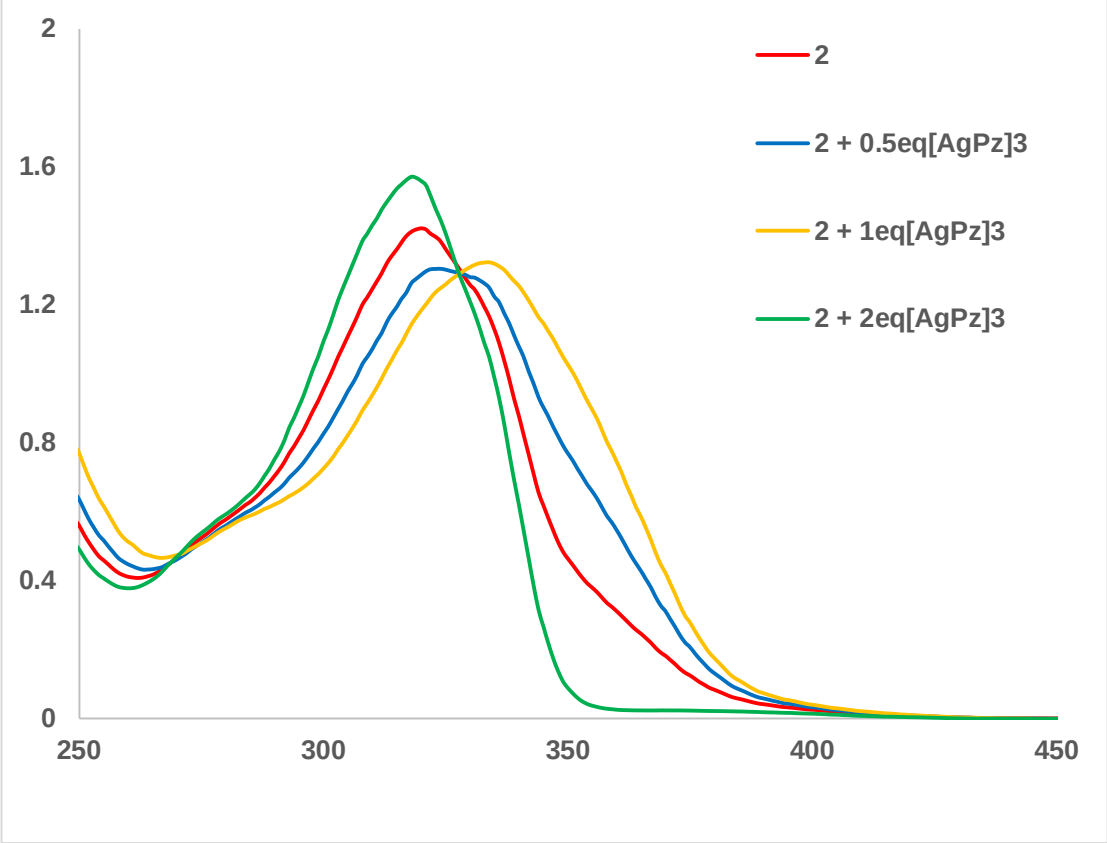


Figure S16. UV-vis spectra of E-**2** + $[AgPz]_3$ c=0.015M d=0.0047cm in CCl_4.

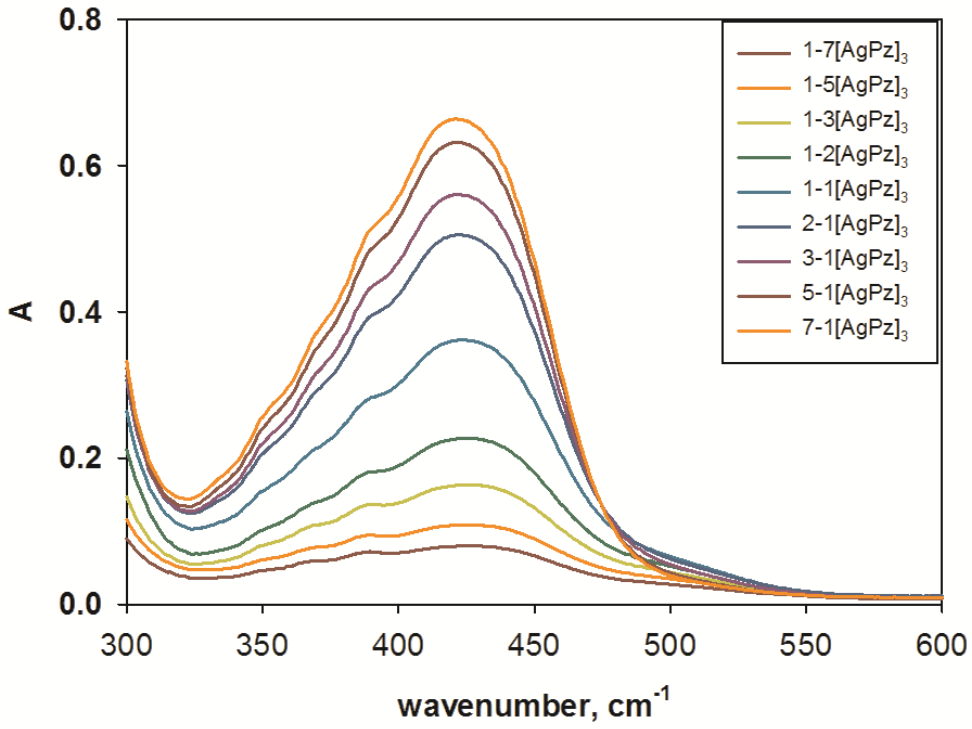


Figure S17. UV-vis spectra of E-**1** + $[AgPz]_3$ c=0.015M d=0.0047cm in CCl_4.

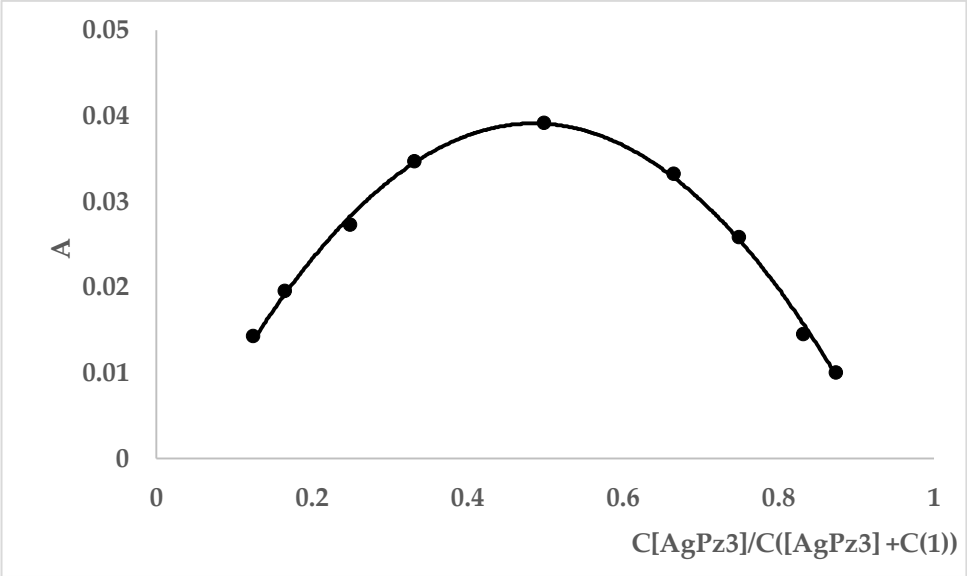


Figure S18. The Job's plot: dependence of the $\nu(CO)^{bond}$ band intensity of $[AgPz]_3$]*[E-**1**] (1674 cm^{-1}) on the composition of the isomolar solution of E-**1** and $[AgPz]_3$, CCl_4.

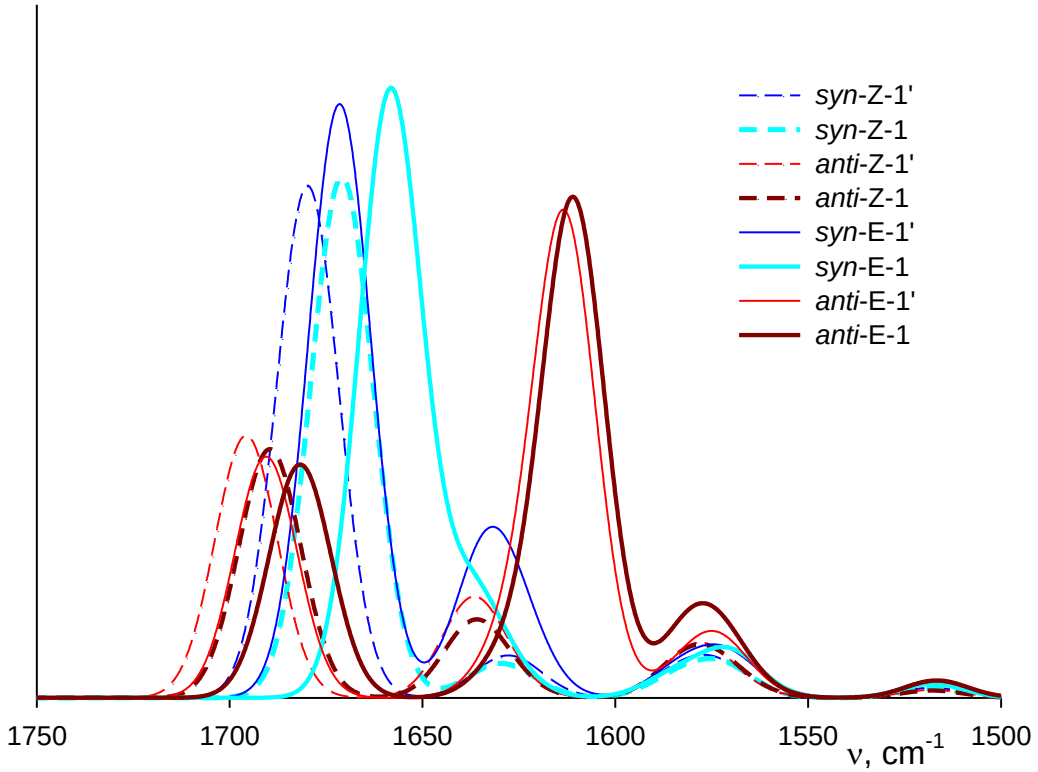


Figure S19. Simulated IR spectra for conformers of chalcone **1**. Frequencies scales by 0.950[1], FWHH set to 19.

Table S2. Coordinates of all optimized species.

syn-Z-**1'** E= -978.116310954947

O	6.853277	6.777755	8.641424
N	5.440236	7.958243	6.534402
C	5.683907	6.518786	8.451021
C	4.835498	7.423084	7.594655
C	3.673545	4.769121	4.783668
C	5.085328	5.319370	9.091946
H	5.516235	5.078614	10.058040
C	3.557544	4.598313	7.221717
C	4.724738	8.760471	5.756319
H	5.232735	9.168059	4.888183
C	3.397721	9.084538	6.007878
H	2.862595	9.744266	5.337206
C	3.519524	7.694736	7.936084
H	3.075910	7.243490	8.813983
C	4.191749	4.488975	8.554373
H	3.895725	3.632219	9.154568
C	4.324431	4.587744	6.044851
C	2.158950	4.718864	7.154894
C	0.102885	5.037719	5.837482
H	-0.364685	5.161645	4.866961
C	2.294201	4.916746	4.734165
H	1.809603	5.059557	3.773920
C	4.459179	4.800984	3.589581
H	3.948352	4.951788	2.645088
C	5.742989	4.392596	6.037291
H	6.257301	4.210316	6.971144
C	1.521680	4.883738	5.889644
C	-0.641059	5.034131	6.971500
H	-1.716702	5.153103	6.921686
C	-0.009178	4.880488	8.236118
H	-0.612060	4.885719	9.136446
C	1.337832	4.733539	8.325444
H	1.800410	4.633538	9.299638
C	2.787839	8.549142	7.127278
H	1.757090	8.781801	7.365163
C	5.803823	4.641631	3.633921
H	6.390110	4.667255	2.723305
C	6.451745	4.422848	4.881188
H	7.524425	4.272683	4.904368

syn-Z-**1** E=-978.117679404354

O	0.458939	-2.332467	-1.597042
N	1.387223	0.963937	-1.221912
C	0.690995	-1.336656	-0.940532
C	0.509409	0.022034	-1.558243
C	-2.193227	1.594571	0.942807
C	1.151810	-1.474084	0.463687
H	1.755852	-2.357789	0.640667
C	-0.082836	0.476436	1.477111
C	1.236323	2.167951	-1.763128
H	1.969988	2.916596	-1.482124
C	0.201773	2.486952	-2.630740
H	0.114125	3.491516	-3.024107
C	-0.538765	0.231363	-2.442598
H	-1.216482	-0.577873	-2.679857
C	0.794731	-0.714379	1.498603
H	1.186770	-0.998543	2.471880
C	-1.410696	0.399309	1.026540
C	0.444639	1.702961	1.916413
C	0.194439	4.123779	2.296631
H	-0.431328	5.008327	2.251720
C	-1.652954	2.803235	1.359800
H	-2.252832	3.705067	1.294135
C	-3.522669	1.524289	0.420654
H	-4.092749	2.443971	0.349652
C	-2.035234	-0.830602	0.639891
H	-1.486635	-1.757374	0.740927
C	-0.357996	2.880948	1.860551
C	1.469311	4.197783	2.753377
H	1.879179	5.144173	3.085219
C	2.279862	3.029820	2.791805
H	3.301389	3.103139	3.145501
C	1.789693	1.830894	2.384009
H	2.429352	0.957478	2.403849
C	-0.702742	1.497357	-2.977605
H	-1.522613	1.708104	-3.653272
C	-4.057916	0.342819	0.028863
H	-5.065171	0.300662	-0.367628
C	-3.302156	-0.856014	0.156332
H	-3.748985	-1.800042	-0.131936

anti-Z-**1'** E= -978.111588000679

O	4.747352	7.370865	8.250632
N	7.306648	8.167610	8.823360
C	5.513867	6.553536	8.708363
C	6.979432	6.874702	8.868249
C	3.657063	5.154290	4.740336
C	5.058727	5.202387	9.135877
H	5.488435	4.804995	10.048951
C	3.549699	4.817861	7.160814
C	8.588221	8.486840	8.923656
H	8.825182	9.545712	8.893419
C	9.603363	7.546081	9.058822
H	10.634794	7.866814	9.128793
C	7.919868	5.864549	9.009796
H	7.616750	4.825807	9.035525
C	4.178966	4.470685	8.458375
H	3.893171	3.510071	8.880718
C	4.302823	4.838104	5.977022
C	2.172024	5.080108	7.128143
C	0.132864	5.648742	5.871147
H	-0.336761	5.872857	4.919739
C	2.293374	5.416629	4.721218
H	1.810201	5.652801	3.778846
C	4.431745	5.191839	3.539101
H	3.925826	5.439464	2.612442
C	5.703931	4.544977	5.940561
H	6.209532	4.272224	6.857310
C	1.536233	5.381128	5.886363
C	-0.594157	5.625078	7.015724
H	-1.657970	5.829011	6.993119
C	0.038894	5.340346	8.257519
H	-0.550691	5.336877	9.166630
C	1.370075	5.080650	8.312446
H	1.839683	4.880327	9.267923
C	9.260613	6.209053	9.099761
H	10.018910	5.442746	9.203029
C	5.760152	4.924755	3.554704
H	6.337234	4.956180	2.638326
C	6.403416	4.590500	4.779013
H	7.463020	4.363874	4.778883

anti-Z-**1** E= -978.115303067927

O	1.600760	0.009100	-1.296322
N	0.962296	-3.440687	-1.003810
C	1.482861	-1.087378	-0.792105
C	1.136044	-2.280964	-1.637578
C	-1.926462	1.488806	0.431116
C	1.658437	-1.310148	0.668242
H	2.253889	-2.164847	0.964675
C	0.169353	0.590312	1.319894
C	0.619230	-4.497730	-1.729794
H	0.484405	-5.430224	-1.191620
C	0.433778	-4.446389	-3.104586
H	0.150549	-5.339159	-3.647212
C	0.976290	-2.129693	-3.007253
H	1.125226	-1.159510	-3.461544
C	1.089619	-0.540447	1.591080
H	1.294886	-0.762279	2.635199
C	-1.083243	0.371383	0.723968
C	0.566010	1.888612	1.673920
C	0.137352	4.312678	1.737724
H	-0.522236	5.142840	1.510066
C	-1.511037	2.771790	0.763683
H	-2.153474	3.615287	0.533014
C	-3.186428	1.264053	-0.206495
H	-3.807284	2.124427	-0.430668
C	-1.570477	-0.934343	0.393329
H	-0.968710	-1.799981	0.636803
C	-0.289621	2.994803	1.388381
C	1.335704	4.521666	2.336903
H	1.648974	5.525044	2.599280
C	2.192931	3.422063	2.620379
H	3.150541	3.601961	3.094500
C	1.826434	2.156224	2.295055
H	2.498594	1.332930	2.503745
C	0.617464	-3.238197	-3.754908
H	0.480121	-3.158565	-4.826328
C	-3.597008	0.011771	-0.522399
H	-4.553864	-0.145889	-1.005492
C	-2.775314	-1.106024	-0.206371
H	-3.120140	-2.105609	-0.443241

syn-E-**1'** E= -978.114299489491

O	2.715734	2.687880	1.169455
N	4.204148	1.225322	-0.762750
C	2.342393	1.623722	0.719345
C	3.343361	0.680716	0.097044
C	-3.450247	0.548853	-0.121556
C	0.921752	1.233968	0.787466
H	0.335049	1.771125	1.524797
C	-1.064641	-0.003435	-0.087535
C	5.132927	0.435262	-1.288449
H	5.810993	0.898430	-1.998150
C	5.264165	-0.909408	-0.968322
H	6.048991	-1.500405	-1.422384
C	3.386752	-0.653784	0.474344
H	2.670102	-1.045839	1.184649
C	0.362463	0.363345	-0.053595
H	1.000408	-0.139276	-0.775061
C	-2.082350	0.969045	-0.124373
C	-1.392942	-1.373439	-0.101722
C	-3.087355	-3.165089	-0.120768
H	-4.134360	-3.447072	-0.132089
C	-3.757880	-0.804883	-0.112160
H	-4.798577	-1.112199	-0.109356
C	-4.488443	1.531522	-0.139237
H	-5.516770	1.187944	-0.120894
C	-1.827148	2.376039	-0.209205
H	-0.807150	2.727700	-0.267292
C	-2.762430	-1.774165	-0.114877
C	-2.113894	-4.108510	-0.111210
H	-2.368664	-5.161418	-0.117450
C	-0.747764	-3.716103	-0.086065
H	0.023655	-4.476783	-0.070195
C	-0.400204	-2.403522	-0.074181
H	0.648366	-2.137643	-0.038965
C	4.377140	-1.461233	-0.062108
H	4.448782	-2.503899	0.222282
C	-4.197721	2.853630	-0.186367
H	-4.991106	3.591019	-0.201123
C	-2.841012	3.277241	-0.237120
H	-2.616706	4.334912	-0.307699

syn-E-**1** E= -978.116260465452

O	2.681561	2.480427	1.632267
N	3.302423	-0.615907	0.225895
C	2.353138	1.488049	1.008225
C	3.407911	0.712380	0.261914
C	-3.398131	0.544530	-0.184346
C	0.938868	1.077530	0.974451
H	0.322183	1.553460	1.730298
C	-1.032912	-0.061276	-0.020711
C	4.261396	-1.296415	-0.393729
H	4.157243	-2.376574	-0.396933
C	5.343931	-0.692283	-1.015425
H	6.089582	-1.296497	-1.515943
C	4.460706	1.406686	-0.318506
H	4.497674	2.485774	-0.251268
C	0.401482	0.278024	0.054368
H	1.049114	-0.185862	-0.681872
C	-2.021372	0.931717	-0.138201
C	-1.392316	-1.420600	0.010433
C	-3.122314	-3.174256	0.005328
H	-4.173467	-3.437702	-0.035046
C	-3.740056	-0.800230	-0.129572
H	-4.787192	-1.083245	-0.160682
C	-4.405766	1.552753	-0.297405
H	-5.443374	1.238406	-0.318987
C	-1.721212	2.327448	-0.255757
H	-0.688463	2.646913	-0.262845
C	-2.769112	-1.790988	-0.041905
C	-2.168967	-4.133679	0.101574
H	-2.446061	-5.180459	0.136481
C	-0.795831	-3.768734	0.164654
H	-0.043587	-4.543509	0.253431
C	-0.420651	-2.464395	0.126881
H	0.629979	-2.209366	0.196498
C	5.442096	0.688303	-0.979192
H	6.271166	1.197352	-1.455343
C	-4.075298	2.863690	-0.384059
H	-4.845787	3.619765	-0.475372
C	-2.706701	3.252292	-0.373212
H	-2.451223	4.301107	-0.467037

anti-E-**1'** E= -978.114505543693

O	2.459365	1.925789	-1.370075
N	4.674743	1.397618	0.213478
C	2.417548	1.030740	-0.552052
C	3.691291	0.509122	0.064122
C	-3.643635	0.584066	0.334321
C	1.148911	0.404242	-0.115558
H	1.180344	-0.284622	0.719679
C	-1.321097	0.164816	-0.331469
C	5.824089	0.969978	0.718208
H	6.600098	1.717649	0.848713
C	6.060207	-0.353763	1.067948
H	7.023884	-0.649064	1.462441
C	3.824579	-0.830778	0.400313
H	3.005268	-1.523626	0.256955
C	-0.004393	0.707001	-0.709655
H	0.023334	1.433432	-1.517956
C	-2.362042	1.072543	-0.059807
C	-1.550762	-1.221548	-0.251050
C	-3.070385	-3.101423	0.255704
H	-4.048363	-3.436270	0.583210
C	-3.848605	-0.785981	0.444125
H	-4.820027	-1.154587	0.757026
C	-4.689944	1.513939	0.618905
H	-5.656514	1.123370	0.917138
C	-2.181181	2.489922	-0.131660
H	-1.213122	2.891608	-0.402654
C	-2.838166	-1.694092	0.157237
C	-2.100479	-3.993366	-0.058677
H	-2.286553	-5.057881	0.016944
C	-0.832635	-3.530696	-0.508191
H	-0.072570	-4.250809	-0.787114
C	-0.567928	-2.203230	-0.600879
H	0.397609	-1.877818	-0.961848
C	5.041607	-1.272148	0.897485
H	5.186576	-2.315588	1.148761
C	-4.479932	2.850033	0.523719
H	-5.278700	3.548871	0.740983
C	-3.201671	3.342504	0.142371
H	-3.042407	4.412194	0.075877

anti-E-**1** E= -978.118736495489

O	2.464032	1.780112	-1.597164
N	3.613440	-0.391400	0.936691
C	2.427803	0.942601	-0.715711
C	3.703067	0.520608	-0.031880
C	-3.586926	0.544881	0.405830
C	1.171526	0.307552	-0.266393
H	1.240703	-0.433461	0.517490
C	-1.308630	0.123196	-0.398904
C	4.732538	-0.766435	1.544127
H	4.628300	-1.509111	2.328440
C	5.981456	-0.257878	1.216801
H	6.862198	-0.600556	1.744463
C	4.907165	1.085720	-0.430326
H	4.918181	1.819471	-1.224632
C	0.002643	0.665014	-0.797139
H	0.010016	1.443878	-1.555436
C	-2.316751	1.032009	-0.025664
C	-1.564125	-1.260932	-0.387287
C	-3.096251	-3.139574	0.083702
H	-4.064026	-3.476237	0.438698
C	-3.814965	-0.825325	0.448104
H	-4.776687	-1.194017	0.789722
C	-4.596758	1.476009	0.798442
H	-5.554326	1.086513	1.125847
C	-2.111074	2.447834	-0.028615
H	-1.150807	2.846708	-0.329448
C	-2.839908	-1.733277	0.056201
C	-2.160701	-4.028294	-0.329310
H	-2.365134	-5.091962	-0.306854
C	-0.905916	-3.562781	-0.811585
H	-0.174538	-4.279169	-1.166392
C	-0.618847	-2.236965	-0.840640
H	0.335660	-1.907023	-1.225586
C	6.068738	0.686381	0.208075
H	7.026242	1.103270	-0.079191
C	-4.364479	2.811484	0.766226
H	-5.136217	3.510899	1.064234
C	-3.098102	3.302084	0.344585
H	-2.920693	4.370858	0.327726