

Supporting information

Stereoselective Synthesis of a Novel Series of Dispiro-oxindolopyrrolizidines Embodying Thiazolo[3,2-a]benzimidazole Motif: A Molecular Electron Density Theory Study of the Mechanism of the [3 + 2] Cycloaddition Reaction

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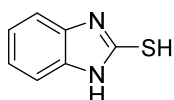
S17 **Figure S20** with $\omega\text{B97X-D/6-311G(d,p)}$ IRC path associated with the most favourable *ortho/endo* reaction path via **TS-CC-on** in ethanol.

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Synthesis of 1*H*-benzo[*d*]imidazole-2-thiol **2**

A mixture of (0.1 mol, 10.8 g) of *o*-phenylenediamine **1**, (0.1 mol, 5.65 g) of potassium hydroxide and (0.1 mol, 7.67 g, 6.19 mL) carbon disulfide, in 90 mL of ethanol in a 250 mL round bottom flask was heated under reflux for 3 h. After completion of heating, reaction mixture was cooled down to room temperature. After that, 100 mL of water were added. The mixture was acidified using diluted acetic acid with stirring. The product was collected by filtration and dried overnight. The dried product was recrystallized from ethanol. White crystals were formed in 96% yield.

1*H*-benzo[*d*]imidazole-2-thiol **2**



Yield (%): 96; White solid material; m.p.: >250 °C; Molecular Formula: C₇H₆N₂S; [M⁺] m/z : 150; ¹H-NMR (400 MHz, DMSO-*d*₆) δ 12.52 (s, 2H, overlapped signals, S-H and N-H), 7.09-7.15 (m, 4H, Ar-H); ¹³C-NMR (101 MHz, DMSO-*d*₆) δ 168.7, 132.8, 122.9, 110.0; Anal. for C₇H₆N₂S; calcd: C, 55.98; H, 4.03; N, 18.65 Found: C, 55.92; H, 4.08; N, 18.70.

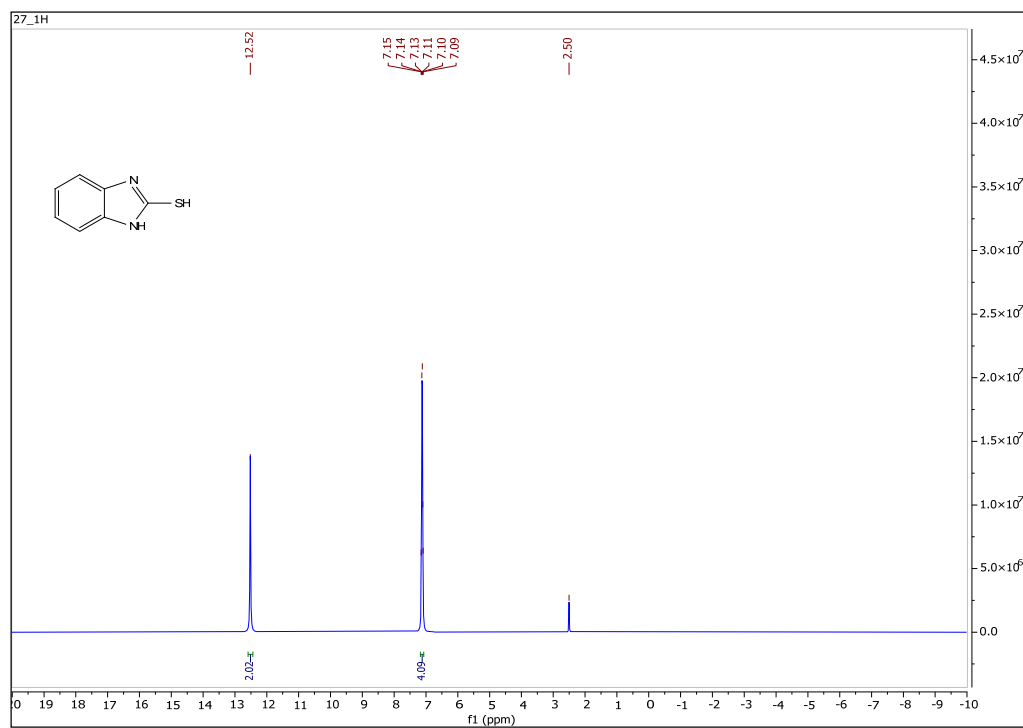


Figure S1: ^1H -NMR Spectrum of compound (2). ($\text{DMSO}-d_6$)

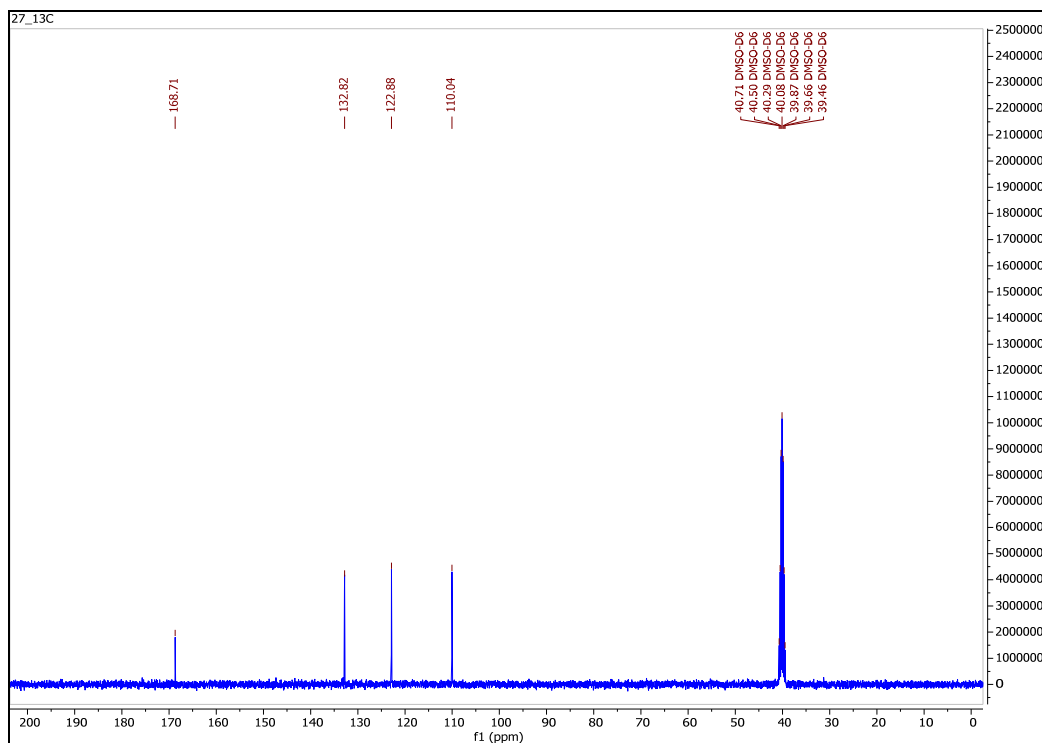


Figure S2: ¹³C-NMR Spectrum of compound (2). (DMSO-*d*₆)

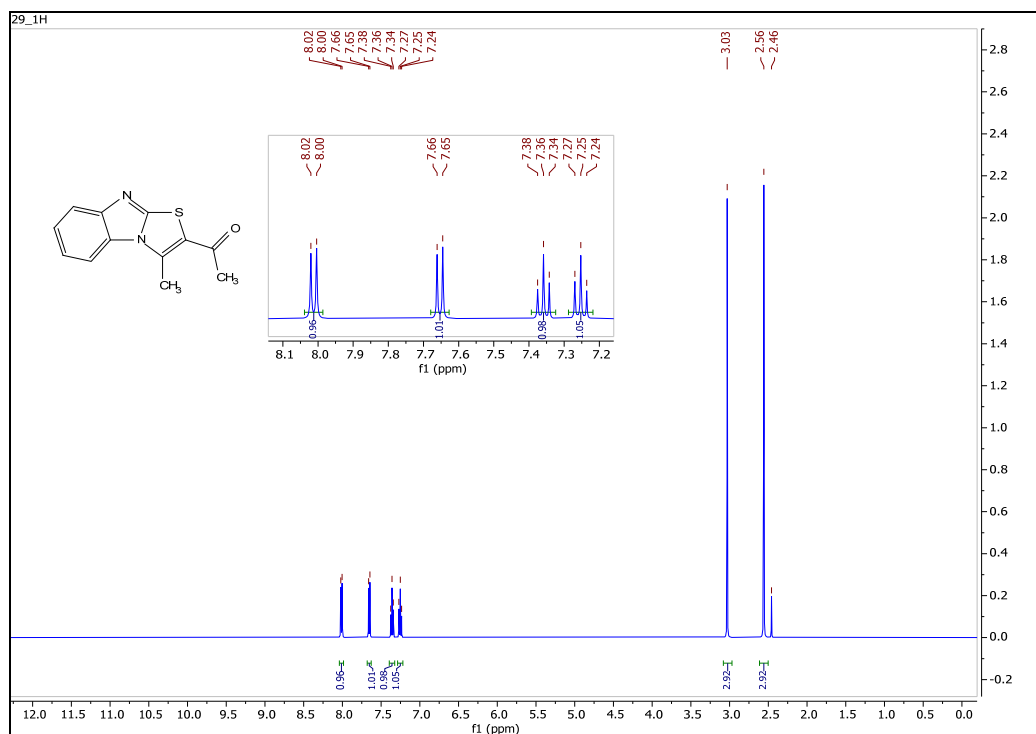


Figure S3: ¹H-NMR Spectrum of compound (4). (DMSO-*d*₆)

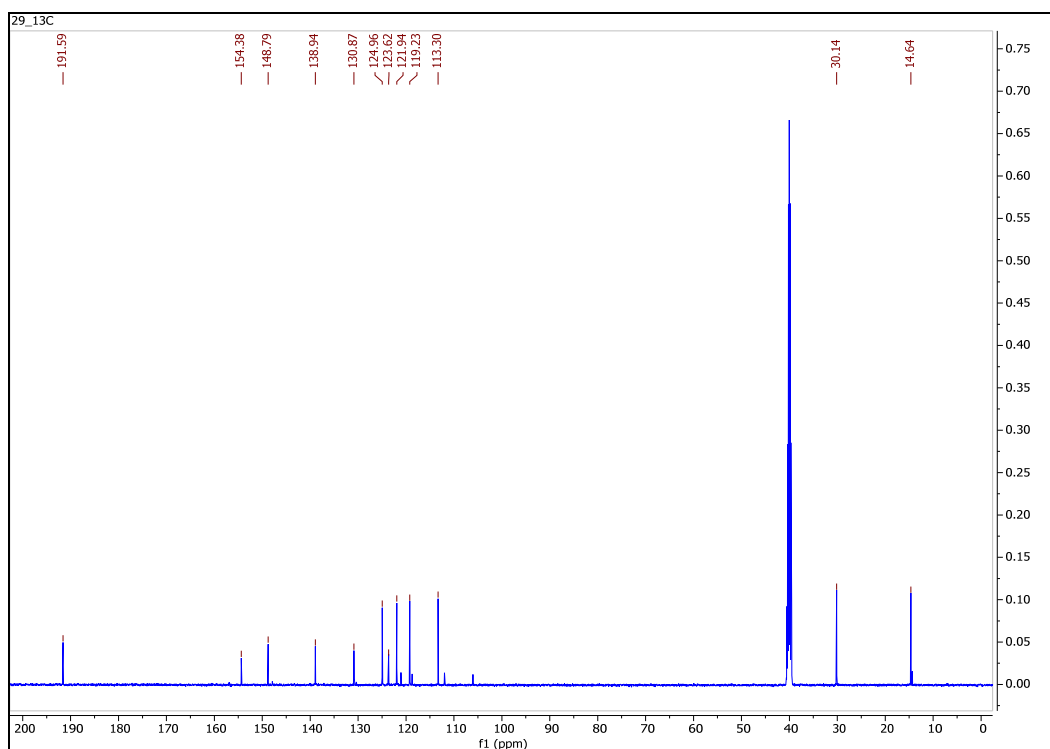


Figure S4: ¹³C-NMR Spectrum of compound (4). (DMSO-*d*₆)

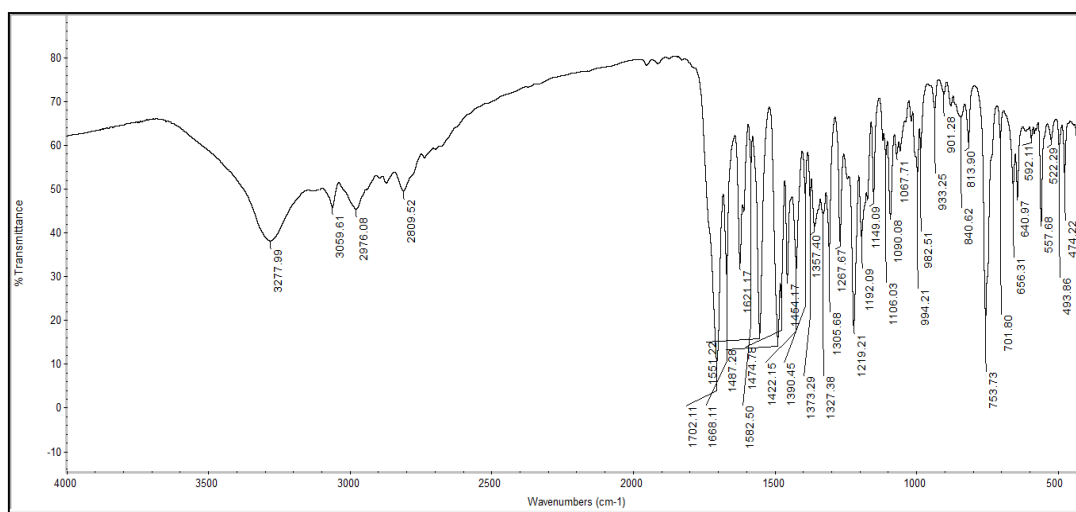


Figure S5: IR Spectrum of compound (6).

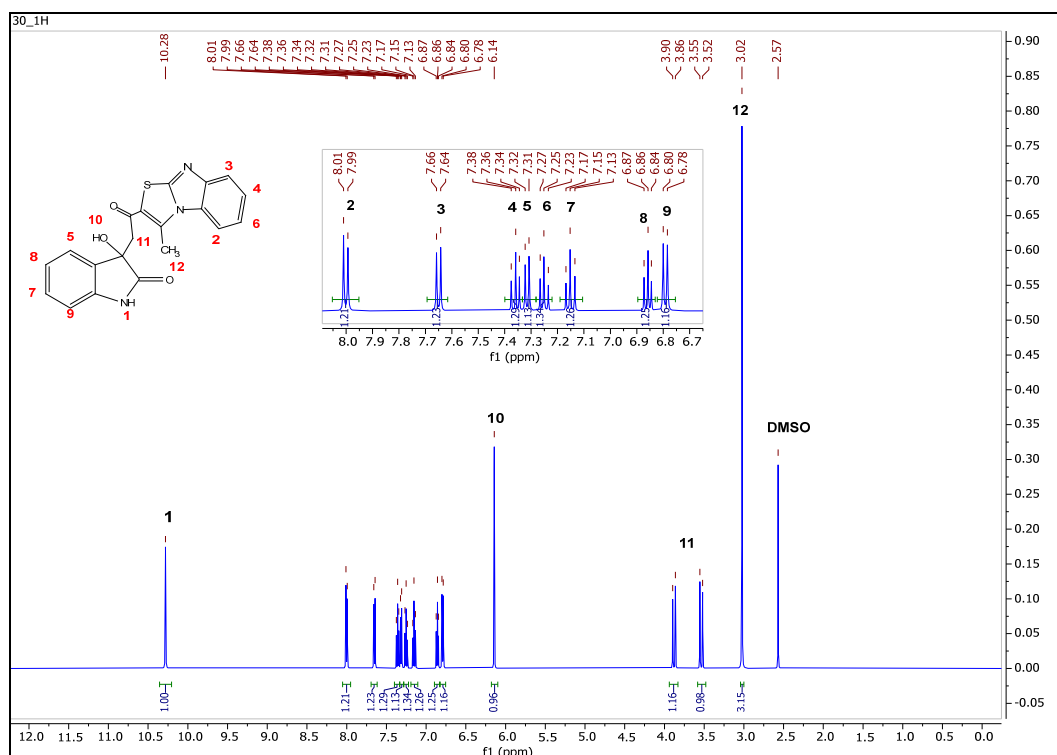


Figure S6: ¹H-NMR Spectrum of compound (6). (DMSO-*d*₆)

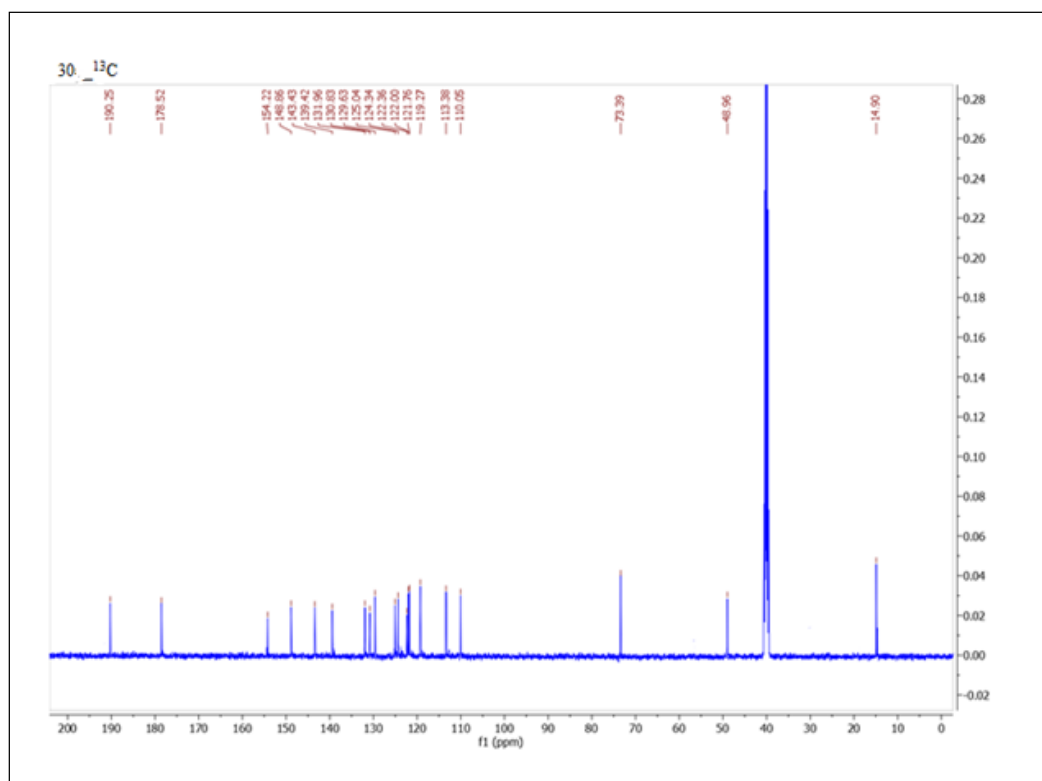


Figure S7: ¹³C-NMR Spectrum of compound (6). (DMSO-*d*₆)

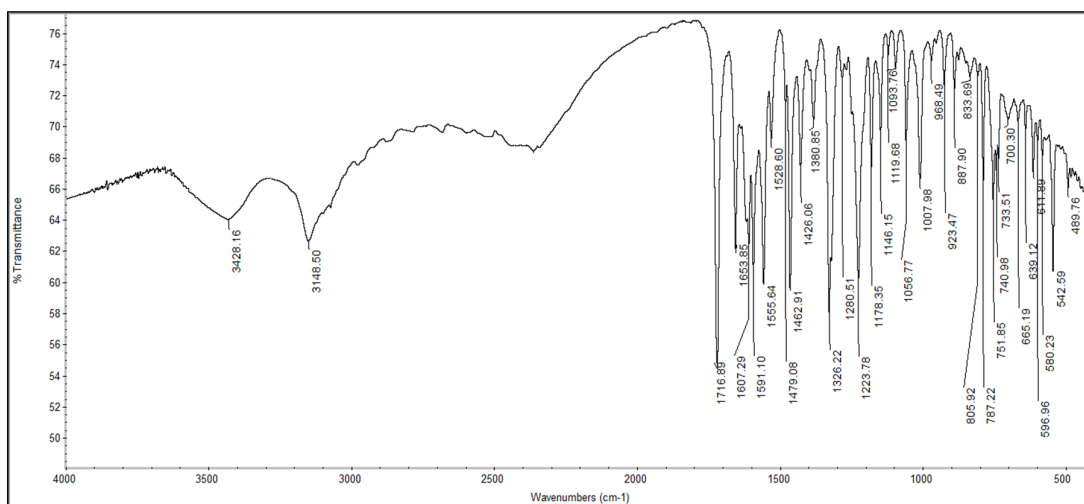


Figure S8: IR Spectrum of compound (7).

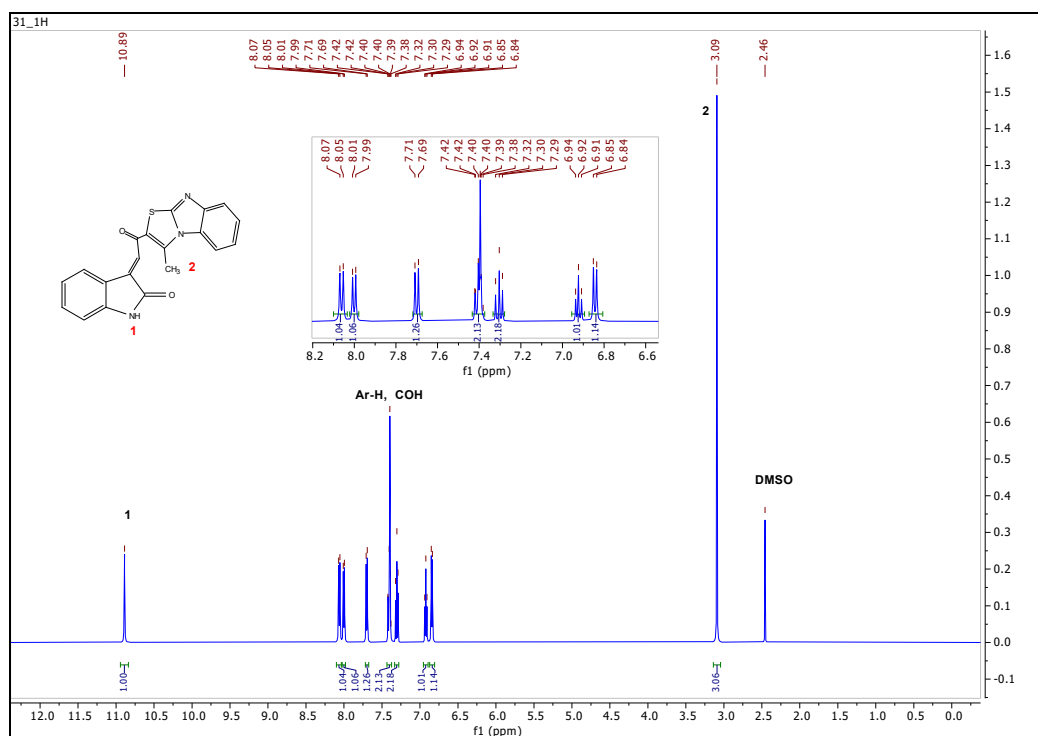


Figure S9: ^1H -NMR Spectrum of compound (7). ($\text{DMSO}-d_6$)

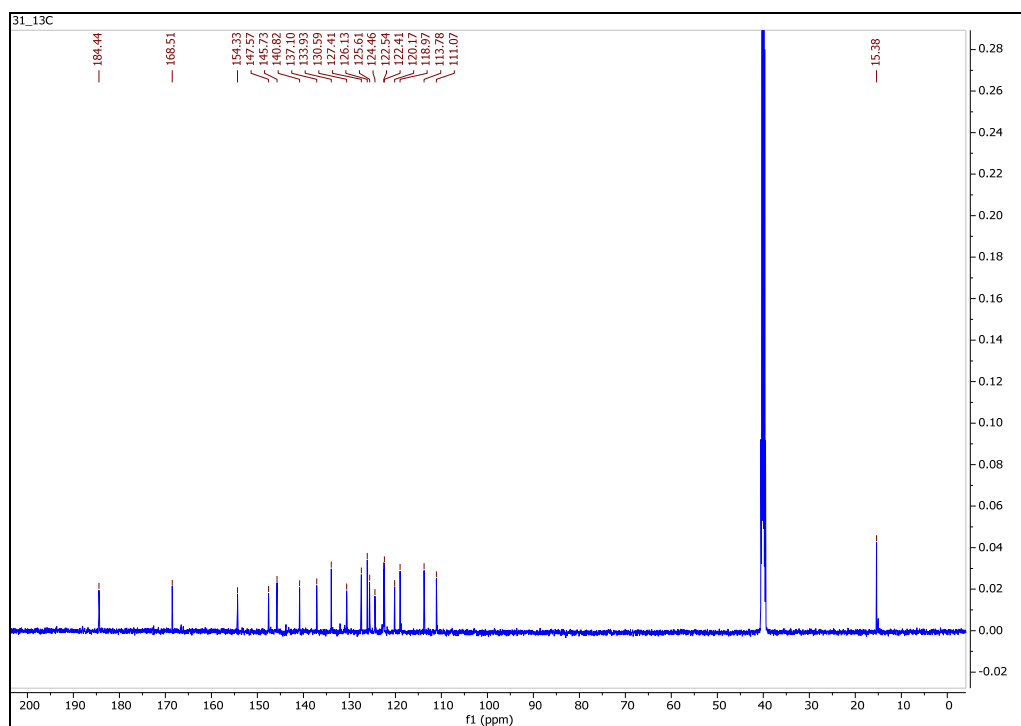


Figure S10: ¹³C-NMR Spectrum of compound (7). (DMSO-*d*₆)

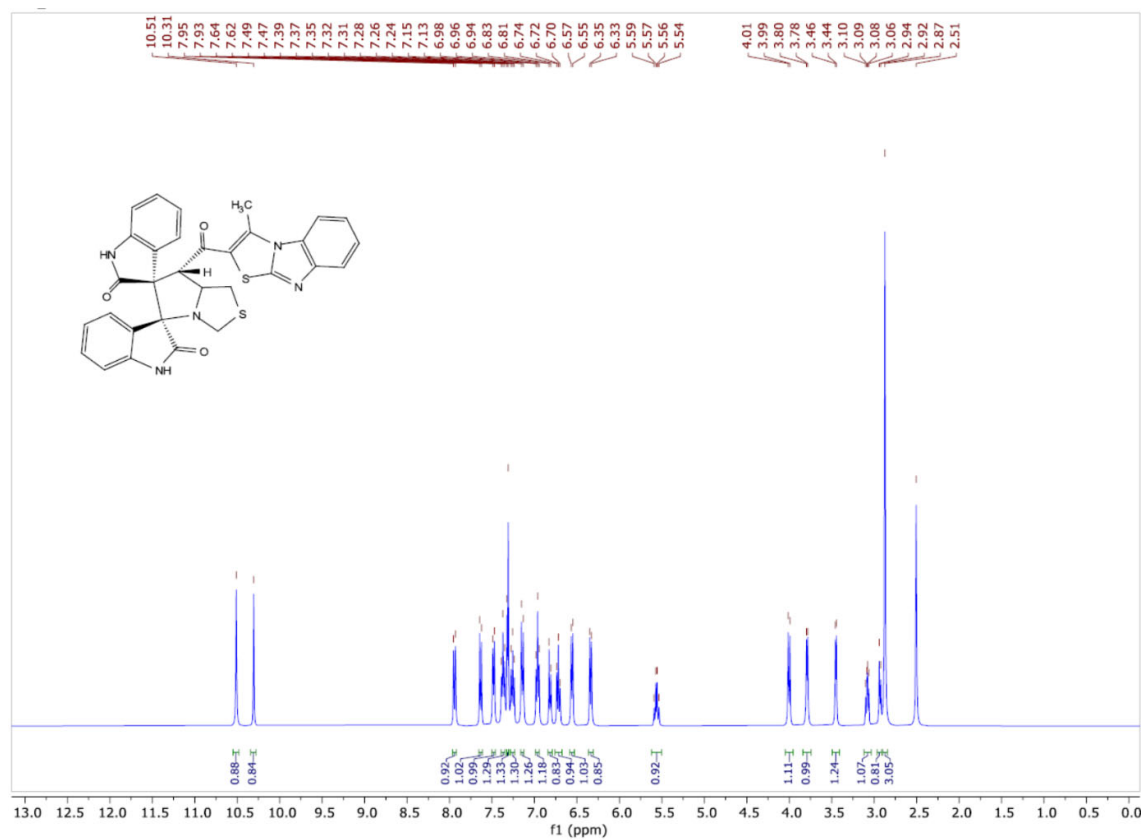


Figure S11: ¹H-NMR Spectrum of compound (9a). (DMSO-*d*₆)

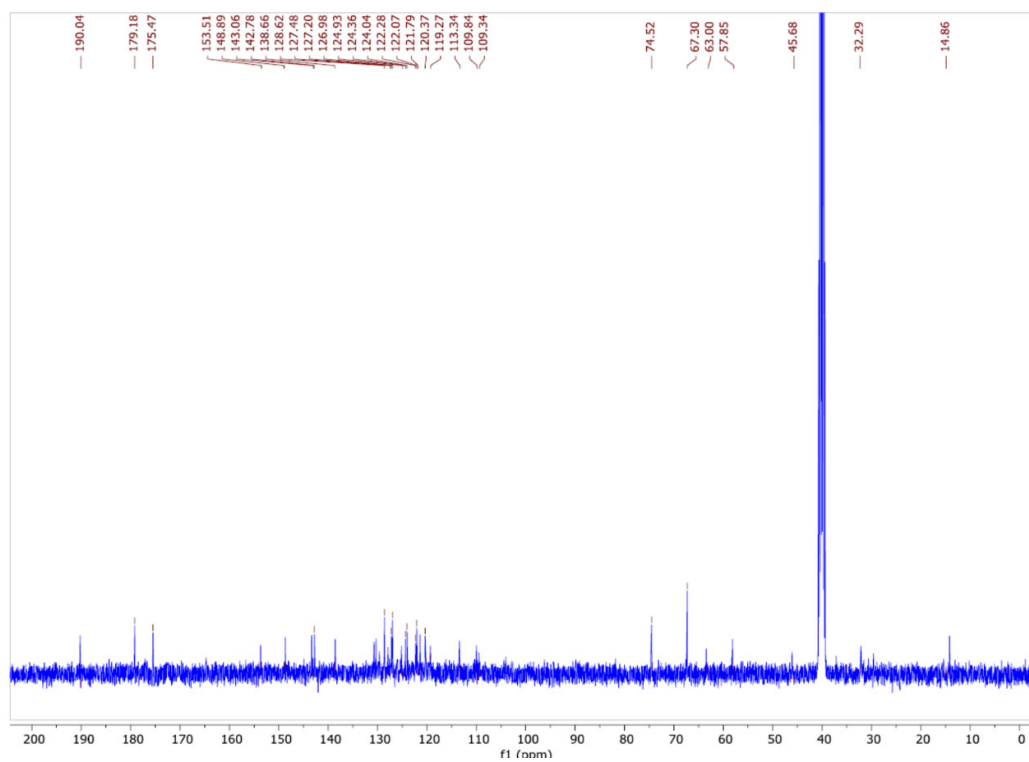


Figure S12: ¹³C-NMR Spectrum of compound (9a). (DMSO-*d*₆)

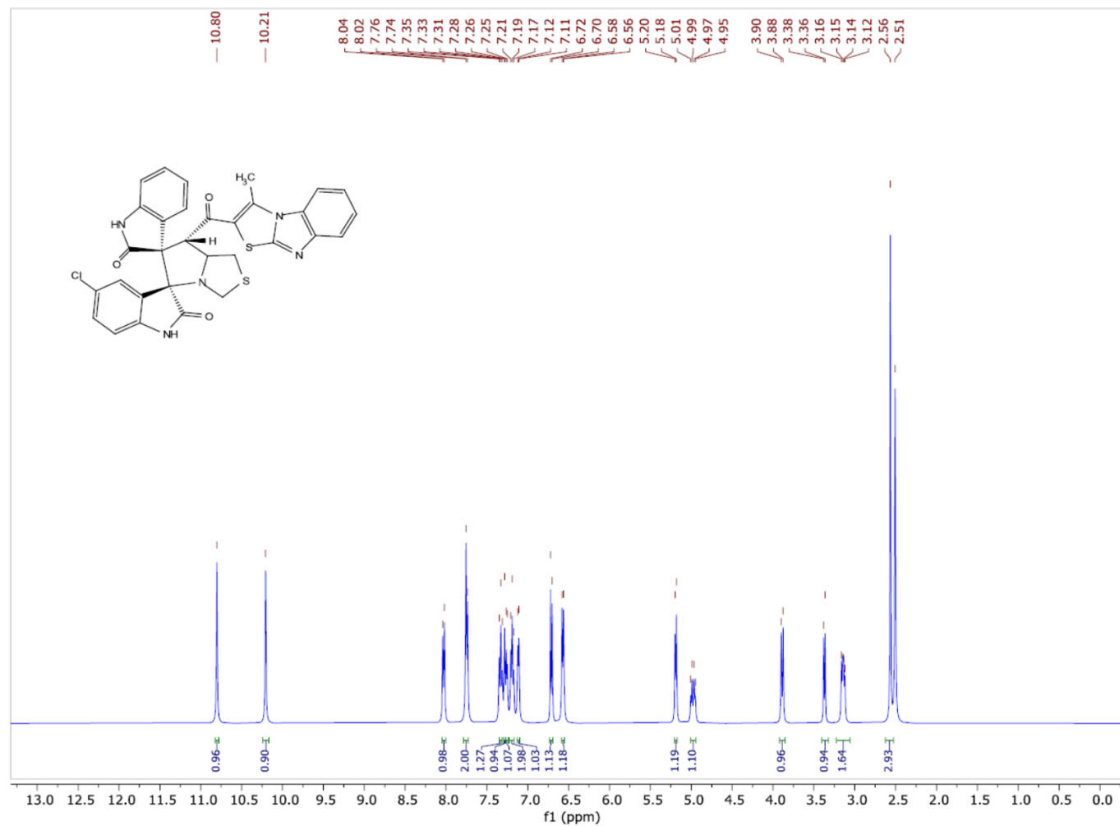
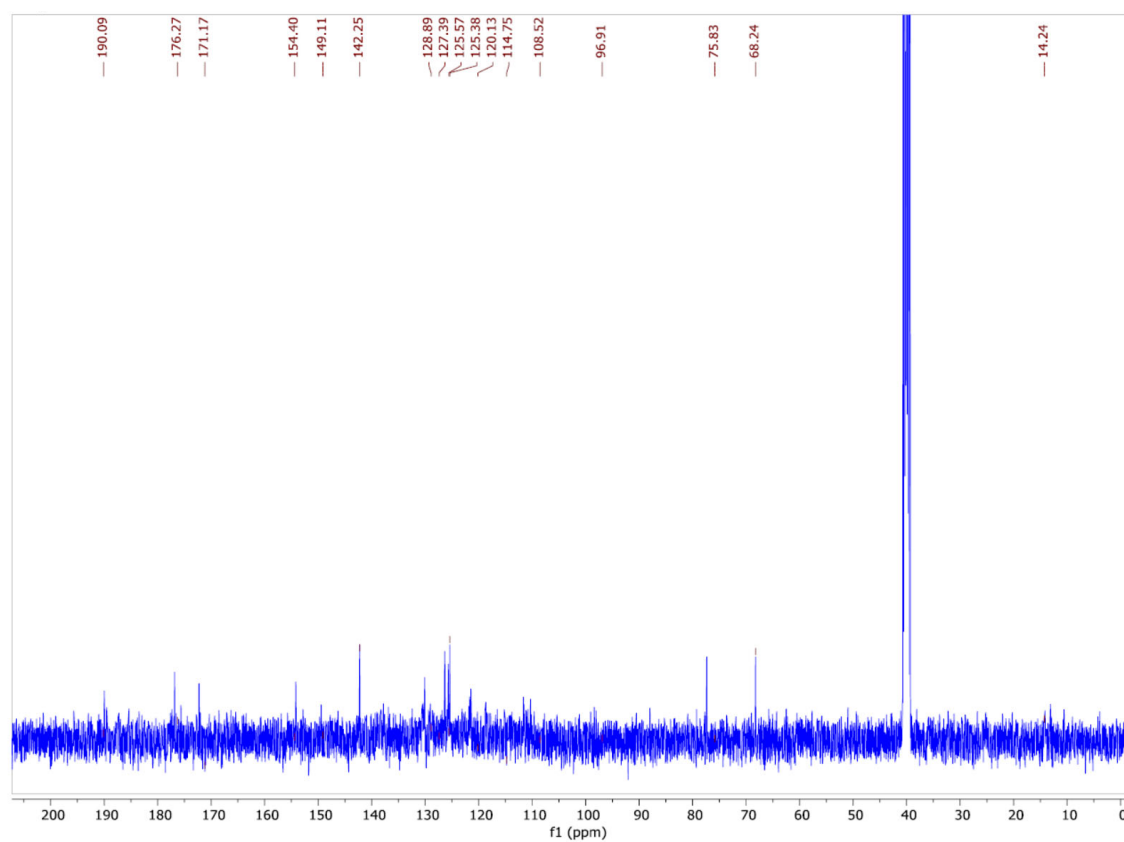
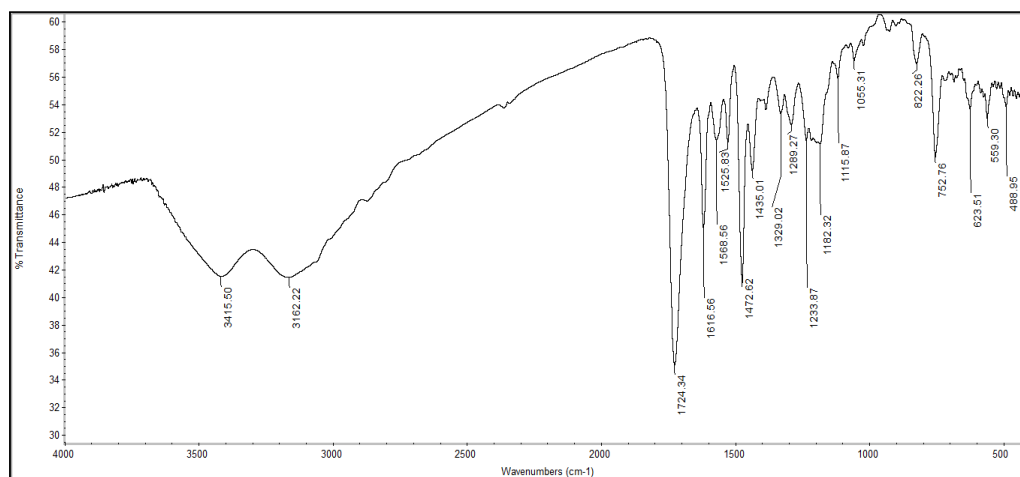


Figure S13: ^1H -NMR Spectrum of compound (**9b**). ($\text{DMSO}-d_6$)**Figure S14:** ^{13}C -NMR Spectrum of compound (**9b**). ($\text{DMSO}-d_6$)**Figure S15:** IR Spectrum of compound (**9c**).

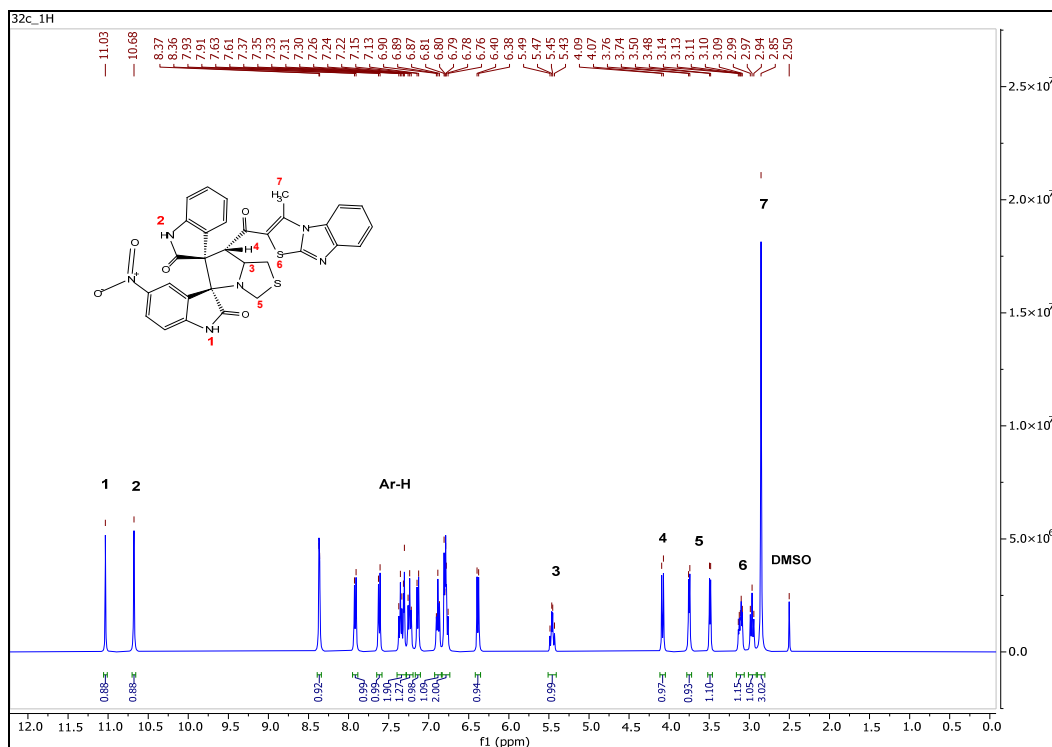


Figure S16: ^1H -NMR Spectrum of compound (9c). (DMSO- d_6)

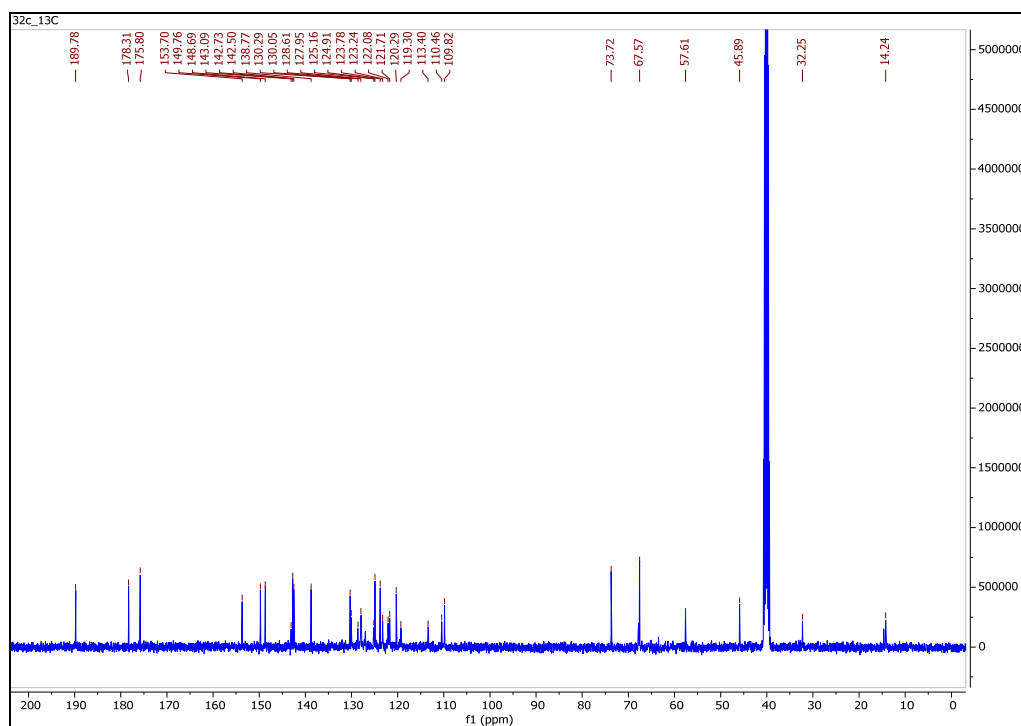


Figure S17: ^{13}C -NMR Spectrum of compound (9c). (DMSO- d_6)

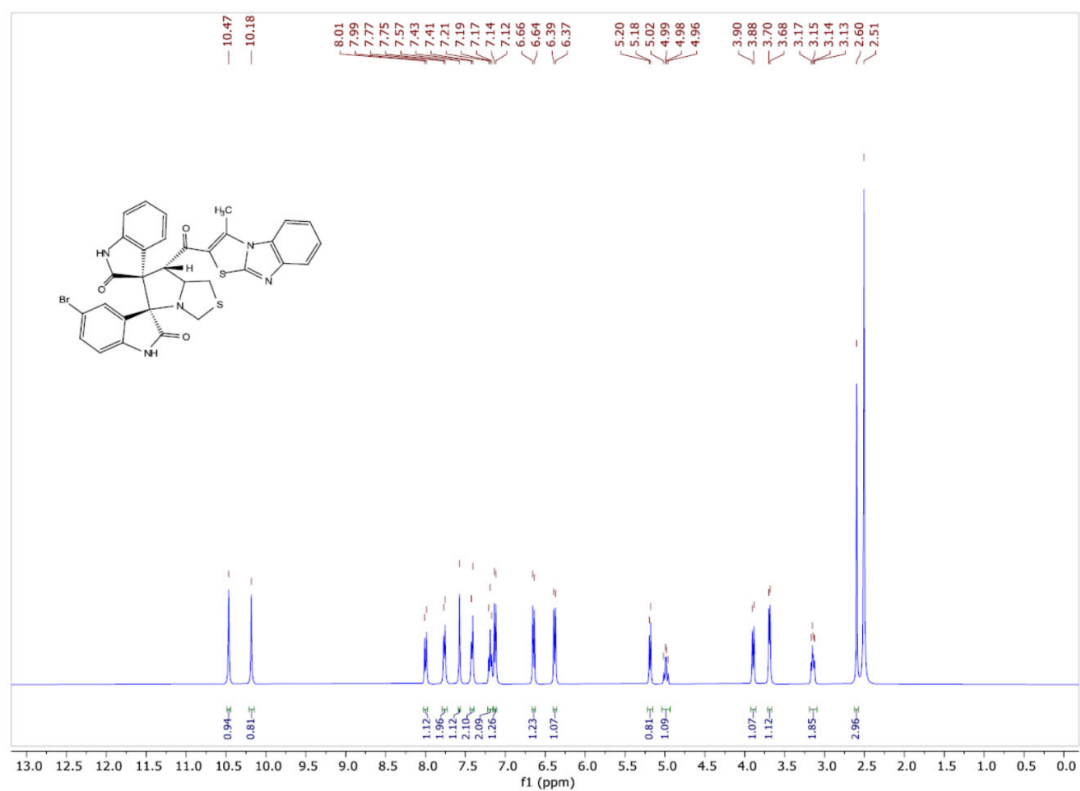


Figure S18: ^1H -NMR Spectrum of compound (9d). (DMSO- d_6)

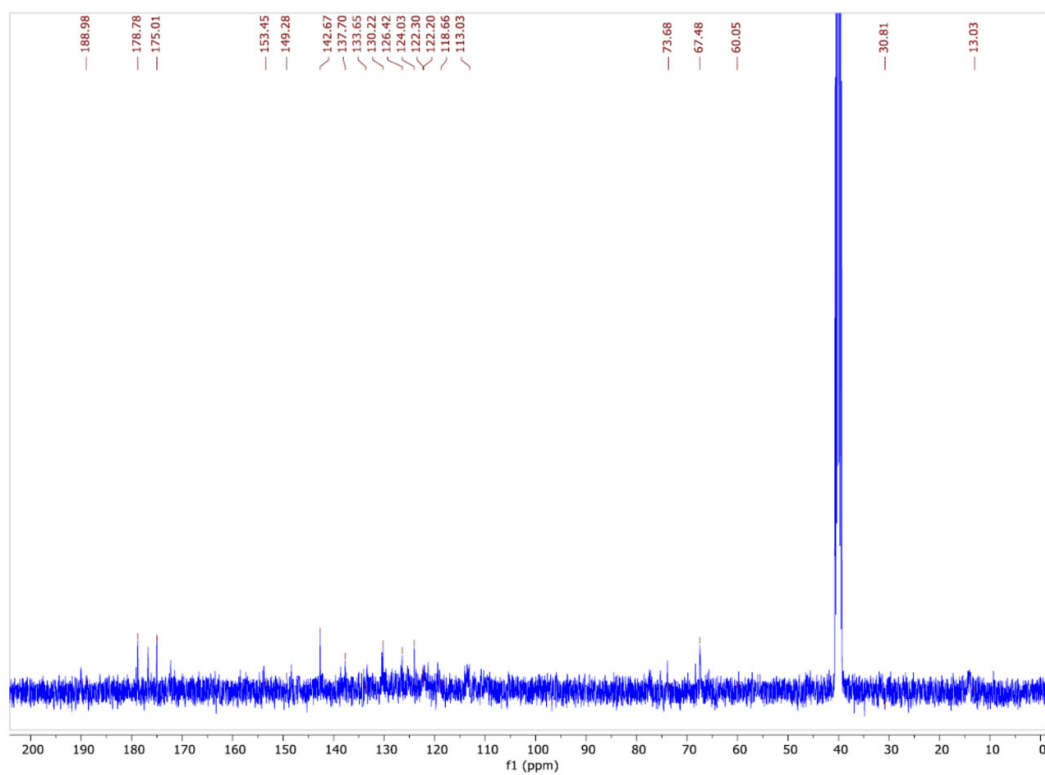


Figure S19: ^{13}C -NMR Spectrum of compound (9d). (DMSO- d_6)

Computational Protocol

All calculations were performed using the ω B97X-D [1] functional together with the standard 6-311G(d,p) [2] basis set. This functional includes long-range exchange and semi classical London dispersion corrections, and has demonstrated to be an efficient method in the study of organic reactions. [3] The TSs were characterized by the presence of only one imaginary frequency. The Berny method was used in optimizations. [4,5] The intrinsic reaction coordinates (IRC) paths [6] were traced to obtain the energy profiles connecting each TS to the two associated minima in the potential energy surface using the Hratchian-Schlegel Hessian-based Predictor-Corrector integrator. [7-9]

Solvent effects of ethanol in the thermodynamic calculations were taken into account by full optimization of the gas-phase structures at the same computational level using the polarizable continuum model (PCM) [10,11] in the framework of the self-consistent reaction field (SCRF). [12-14] Values of ω B97X-D/6-311G(d,p) enthalpies, entropies, and Gibbs free energies in ethanol were calculated with standard statistical thermodynamics at 78 °C and 1 atm [2] by PCM frequency calculations at the solvent-optimized structures.

The GEDT [15] values were computed using the equation $\text{GEDT}(f) = \sum q_f$, where q are the natural charges [16,17] of the atoms belonging to one of the two frameworks (f) at the TS geometries. Quantum chemical reactivity indices [18,19] were calculated using the equations in reference 19.

The Gaussian 16 suite of programs was used to perform the calculations. [20] Molecular geometries were visualized by using the GaussView program. [21]

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Table S1. ω B97X-D/6-311G(d,p) enthalpies (H, in kcal·mol⁻¹), entropies (S, in cal·mol⁻¹·K⁻¹) and Gibbs free energies (G, in kcal·mol⁻¹), and the relative ones with respect to the separated reagents (Δ H, Δ S and Δ G), computed at 78 °C and 1 atm in ethanol, for the stationary points involved in the 32CA reaction of AY **10a** with chalcone **7**.

	H	Δ H	S	Δ S	G	Δ G
chalcone 7	-1482.453114		165.705		-1482.545940	
AY 10a	-1007.834257		117.964		-1007.900338	0.0
MC-CC-mn	-2490.320010	-20.5	236.227	-47.4	-2490.452340	-3.8
TS-CC-on	-2490.309517	-13.9	230.490	-53.2	-2490.438634	4.8
TS-CC-ox	-2490.303704	-10.2	229.317	-54.4	-2490.432164	8.9
TS-CC-mn	-2490.310307	-14.4	226.091	-57.6	-2490.436959	5.8
TS-CC-mx	-2490.305699	-11.5	227.594	-56.1	-2490.433194	8.2
TS-CO-on	-2490.298576	-7.0	227.213	-56.5	-2490.425856	12.8
TS-CO-ox	-2490.296157	-5.5	226.092	-57.6	-2490.422810	14.7
TS-CO-mn	-2490.281194	3.9	230.491	-53.2	-2490.410311	22.6
TS-CO-mx	-2490.285077	1.4	230.980	-52.7	-2490.414468	20.0
9a	-2490.358521	-44.6	224.110	-59.6	-2490.484064	-23.7
11a	-2490.345111	-36.2	222.316	-61.4	-2490.469648	-14.7
12a	-2490.358734	-44.8	222.848	-60.8	-2490.483570	-23.4
13a	-2490.363843	-48.0	226.686	-57.0	-2490.490828	-28.0
14a	-2490.326760	-24.7	227.522	-56.1	-2490.454213	-5.0
15a	-2490.326907	-24.8	227.169	-56.5	-2490.454163	-4.9
16a	-2490.323562	-22.7	230.565	-53.1	-2490.452721	-4.0
17a	-2490.325136	-23.7	227.833	-55.8	-2490.452765	-4.1

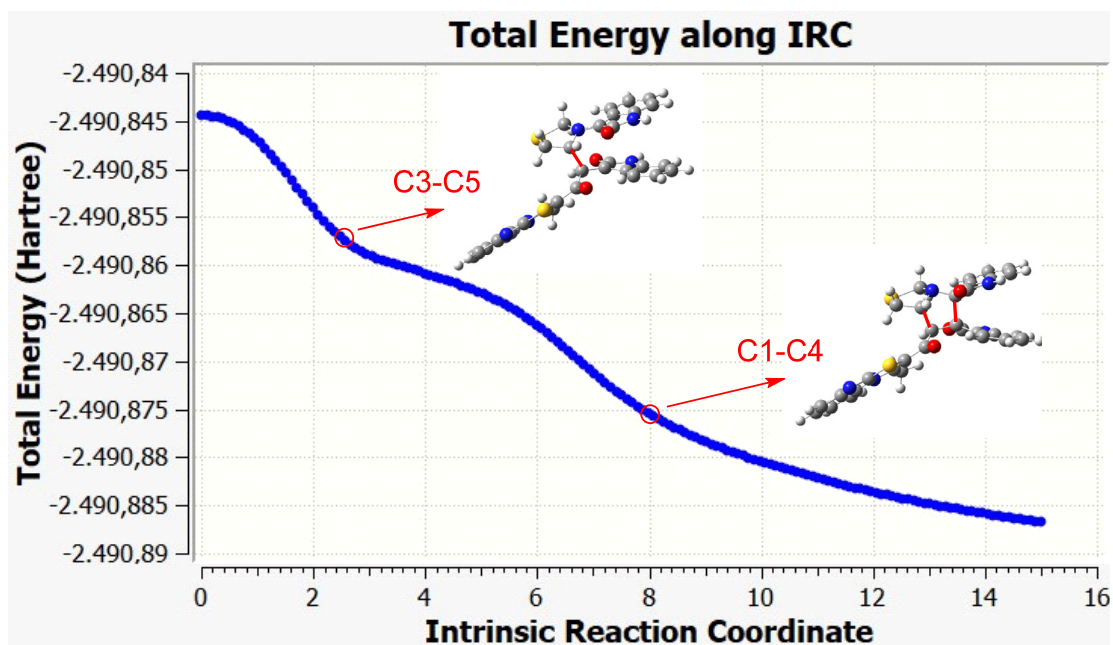


Figure S20. ω B97X-D/6-311G(d,p) IRC path associated with the most favourable *ortho/endo* reaction path via **TS-CC-on** in ethanol.

Cartesian coordinates and electronic energies of the stationary points involved in the 32CA reaction between AY **10a** and chalcone **7** in ethanol. Imaginary frequencies for TSs at 78 °C are included.

Chalcone **7**

E(RwB97XD) = -1482.77380792 A.U.

6	-1.574396	0.395625	-0.878872
1	-1.068688	1.232315	-1.351703
6	-0.793564	-0.847586	-0.695542
8	-1.303503	-1.954294	-0.776049
6	3.988349	0.510076	0.297344
6	4.911184	-0.543918	0.129474
6	3.029530	-1.385913	-0.335218
6	0.653822	-0.737428	-0.483673
6	1.428596	0.304878	-0.071505
6	6.268113	-0.315756	0.356070
6	6.661921	0.956018	0.738619
1	7.711354	1.156812	0.919919
6	4.377559	1.791183	0.672359
6	5.731706	1.993991	0.892578
1	6.075899	2.977987	1.187434
1	6.984132	-1.118729	0.230407
1	3.670590	2.601451	0.785562
16	1.573468	-2.233430	-0.740277
7	2.757536	-0.067646	-0.011915
7	4.280622	-1.720322	-0.267500
6	1.051336	1.680559	0.357663
1	1.407994	2.419637	-0.364851
1	-0.023173	1.787906	0.471328
1	1.513774	1.895417	1.323665
6	-3.898704	-0.168111	0.137479
6	-5.006644	0.688726	0.271168
6	-6.177639	0.287406	0.885038
6	-6.231865	-1.016063	1.377006
6	-5.150261	-1.883295	1.250173
6	-3.977980	-1.467800	0.624116
6	-2.852288	0.598616	-0.536704
6	-3.450733	1.969958	-0.808092
1	-7.021092	0.959867	0.979948
1	-7.138776	-1.358339	1.861999
1	-5.223292	-2.893643	1.633553
1	-3.144133	-2.144215	0.500046
7	-4.716680	1.932000	-0.295357
1	-5.350123	2.714406	-0.330591
8	-2.915065	2.907890	-1.355922

AY 10a

E(RwB97XD) = -1008.04671945 A.U.

6	-1.639347	-1.255089	0.049759
7	-1.284521	0.178145	0.069875
6	0.055644	0.525154	0.034530
6	1.224861	-0.320086	0.030763
6	2.328986	0.569882	-0.050856
6	3.641941	0.131096	-0.072689
6	3.881148	-1.239160	-0.007094
6	2.817762	-2.134291	0.085360
6	1.498090	-1.690351	0.108279
6	0.466292	1.898328	-0.029016
1	4.458520	0.841420	-0.137094
1	0.708609	-2.424739	0.194878
6	-2.288684	1.000936	0.144798
1	-1.343843	-1.691667	1.003192
7	1.850995	1.865206	-0.090873
1	-2.074896	2.060240	0.190010
8	-0.208140	2.937720	-0.039591
1	2.413490	2.697951	-0.137905
1	4.900439	-1.607159	-0.023342
6	-3.648342	0.413203	0.197650
1	-4.082004	0.534841	1.194262
1	3.015400	-3.198649	0.144200
16	-3.431178	-1.347647	-0.226008
1	-4.312787	0.885291	-0.526894
1	-1.114388	-1.738131	-0.770363

MC-CC-mn

E(RwB97XD) = -2490.85614322 A.U.

6	1.112899	-0.774263	-0.817767
1	0.605227	0.044690	-1.310317
6	0.281625	-1.716892	-0.051154
8	0.746979	-2.568334	0.693681
6	-4.536073	-0.455272	-0.992101
6	-5.430632	-0.937610	-0.014156
6	-3.547305	-1.724410	0.529735
6	-1.178449	-1.578983	-0.143937
6	-1.987339	-0.913397	-1.016642
6	-6.773792	-0.565665	-0.063473
6	-7.180235	0.283394	-1.079784
1	-8.218609	0.588704	-1.136049

6	-4.934610	0.406298	-2.007542
6	-6.273840	0.764327	-2.035816
1	-6.623851	1.435284	-2.811119
1	-7.468068	-0.930456	0.683759
1	-4.241698	0.799773	-2.738043
16	-2.079313	-2.407484	1.141480
7	-3.307209	-0.994383	-0.619043
7	-4.783088	-1.734455	0.925890
6	-1.682161	-0.227072	-2.304960
1	-1.730167	0.857952	-2.182237
1	-0.705177	-0.502313	-2.690002
1	-2.423208	-0.524991	-3.049070
6	3.574074	-1.637821	-0.608279
6	4.706435	-1.142834	-1.282043
6	5.964367	-1.686813	-1.112916
6	6.085908	-2.763604	-0.234875
6	4.982232	-3.264322	0.449146
6	3.719165	-2.704596	0.271438
6	2.442713	-0.806873	-1.017129
6	3.011259	0.228300	-1.965298
1	6.823436	-1.289931	-1.639696
1	7.061031	-3.211219	-0.081609
1	5.106013	-4.096488	1.131513
1	2.855741	-3.074881	0.804548
7	4.342671	-0.052384	-2.078730
1	4.967731	0.468009	-2.673718
8	2.410397	1.124003	-2.526638
6	2.050688	3.017686	0.003617
7	2.014468	1.807557	0.847437
6	0.797518	1.320068	1.269606
6	3.172205	1.261648	1.097795
6	-0.533177	1.765439	0.933685
6	-1.395116	1.088533	1.832436
6	-2.771883	1.223363	1.786903
6	-3.317955	2.053533	0.811448
6	-2.493618	2.721380	-0.090972
6	-1.108133	2.583483	-0.041230
6	0.716125	0.385355	2.367059
1	-3.405241	0.681614	2.479859
1	-0.502478	3.102638	-0.772860
1	1.715269	2.738823	-0.994967
7	-0.630760	0.305980	2.677183
1	3.193879	0.347576	1.673848
8	1.610962	-0.223109	2.959142
1	-0.991993	-0.336306	3.362319
1	-4.393991	2.163633	0.744754

6	4.382647	2.000287	0.669848
1	4.951089	1.430895	-0.070081
1	-2.934523	3.353510	-0.853227
16	3.778335	3.581054	-0.014939
1	5.035020	2.195889	1.522537
1	1.407670	3.777797	0.440722

TS-CC-on

E(RwB97XD) = -2490.84443084 A.U.

Imaginary frequency = -347.7547 cm⁻¹

6	0.097988	0.321688	0.106968
1	-0.357831	-0.589254	0.475675
6	-0.834054	1.339815	-0.411010
8	-0.481681	2.333325	-1.028780
6	-5.521793	-0.222643	0.772748
6	-6.517344	0.342399	-0.052573
6	-4.701005	1.179066	-0.733912
6	-2.278333	1.077448	-0.266552
6	-2.984111	0.295539	0.596781
6	-7.852645	-0.015307	0.132876
6	-8.152461	-0.928142	1.130530
1	-9.183183	-1.221299	1.292448
6	-5.814809	-1.148056	1.768739
6	-7.148952	-1.487875	1.934561
1	-7.418604	-2.204677	2.700831
1	-8.623749	0.414012	-0.495148
1	-5.048838	-1.594962	2.387296
16	-3.310397	1.958875	-1.411387
7	-4.336735	0.345442	0.308008
7	-5.972823	1.217529	-0.987950
6	-2.540574	-0.493488	1.781743
1	-2.605730	-1.566208	1.580009
1	-1.522789	-0.250901	2.071939
1	-3.192131	-0.263318	2.627311
6	2.220797	1.735927	0.769430
6	3.237080	1.397808	1.687774
6	4.296932	2.240623	1.962346
6	4.339725	3.462504	1.291962
6	3.347429	3.817432	0.381390
6	2.284006	2.959181	0.109811
6	1.336176	0.583122	0.679011
6	1.872590	-0.427722	1.636133
1	5.070548	1.955586	2.665085
1	5.161644	4.142915	1.483718

1	3.406170	4.771497	-0.129396
1	1.522919	3.215954	-0.611915
7	2.986406	0.129998	2.204818
1	3.607798	-0.385706	2.806587
8	1.420737	-1.535085	1.892770
6	1.155674	-2.781691	-1.066413
7	1.500680	-1.397897	-1.441129
6	2.706958	-0.874778	-1.115875
6	0.472495	-0.626531	-1.826966
6	3.823506	-1.476787	-0.413304
6	4.865694	-0.524629	-0.468080
6	6.062209	-0.693182	0.203411
6	6.232714	-1.859633	0.943667
6	5.229268	-2.824363	0.996272
6	4.024102	-2.643456	0.325156
6	3.185564	0.391394	-1.713379
1	6.837021	0.062109	0.153109
1	3.268527	-3.412115	0.392211
1	1.352546	-2.922907	-0.007528
7	4.471817	0.541174	-1.261399
1	0.723291	0.319180	-2.287719
8	2.609469	1.170228	-2.459087
1	4.997004	1.388051	-1.405723
1	7.161193	-2.019111	1.479287
6	-0.731779	-1.394950	-2.257479
1	-1.658466	-0.884705	-1.996640
1	5.385005	-3.730985	1.568487
16	-0.634619	-2.966404	-1.341376
1	-0.715162	-1.562125	-3.336892
1	1.741165	-3.466335	-1.679064

TS-CC-ox

E(RwB97XD) = -2490.83862303 A.U.

Imaginary frequency = -355.8283 cm⁻¹

6	-0.025167	-0.211074	-0.296362
1	-0.554823	-0.668915	-1.122458
6	-0.859615	0.541577	0.658975
8	-0.404872	1.335327	1.472272
6	-5.689944	-0.813688	-0.120770
6	-6.615734	0.131743	0.369601
6	-4.716892	0.929431	0.840635
6	-2.321256	0.395516	0.570931
6	-3.110316	-0.590182	0.060709
6	-7.982832	-0.094127	0.210611

6	-8.383370	-1.252037	-0.435432
1	-9.440583	-1.448328	-0.570738
6	-6.085081	-1.973695	-0.778372
6	-7.449096	-2.176731	-0.924135
1	-7.797632	-3.069157	-1.429893
1	-8.700887	0.625513	0.584570
1	-5.374258	-2.689282	-1.167934
16	-3.248137	1.717534	1.312195
7	-4.448350	-0.268169	0.202161
7	-5.976330	1.214061	0.967381
6	-2.757021	-1.916953	-0.519563
1	-2.977733	-1.940744	-1.590246
1	-1.709359	-2.160124	-0.371474
1	-3.354220	-2.689870	-0.030829
6	1.946846	-0.949011	1.281037
6	2.836250	-2.033562	1.126956
6	3.781017	-2.362031	2.080241
6	3.832945	-1.586767	3.236330
6	2.966740	-0.512968	3.414886
6	2.030600	-0.179548	2.438153
6	1.124083	-0.905796	0.077245
6	1.513776	-2.094470	-0.734019
1	4.456903	-3.195401	1.930914
1	4.563573	-1.823193	4.001422
1	3.026553	0.081895	4.318780
1	1.367790	0.662901	2.577148
7	2.579026	-2.669509	-0.081964
1	3.023013	-3.515329	-0.399257
8	0.985365	-2.517483	-1.748639
6	1.999825	2.688793	-0.105898
7	1.857116	1.606165	-1.087474
6	2.807316	0.652193	-1.225128
6	0.608918	1.434455	-1.560367
6	4.060599	0.509802	-0.520692
6	4.806967	-0.446271	-1.241204
6	6.028923	-0.915359	-0.796485
6	6.520115	-0.407310	0.403675
6	5.800966	0.536662	1.132044
6	4.568125	0.994543	0.683707
6	2.897376	-0.158911	-2.465730
1	6.581310	-1.655172	-1.362963
1	4.017657	1.704898	1.283979
1	2.982470	3.143414	-0.208095
7	4.108890	-0.803815	-2.386417
1	0.522126	0.788018	-2.421203
8	2.113435	-0.237657	-3.396804

1	4.417278	-1.466817	-3.078034
1	7.476360	-0.757148	0.774975
6	-0.253501	2.658759	-1.470333
1	-0.451796	3.052549	-2.467547
1	6.197007	0.908768	2.068939
16	0.711186	3.895548	-0.530096
1	-1.210302	2.461180	-0.987265
1	1.847493	2.290511	0.895712

TS-CC-mn

E(RwB97XD) = -2490.84530809 A.U.

Imaginary frequency = -311.0520 cm⁻¹

6	1.111975	-0.422944	-0.495472
1	0.577044	0.293411	-1.103742
6	0.316028	-1.548046	0.009041
8	0.778344	-2.486126	0.644584
6	-4.497110	-0.375608	-1.079964
6	-5.418380	-0.935244	-0.169274
6	-3.540382	-1.720687	0.394059
6	-1.149444	-1.477140	-0.172227
6	-1.938004	-0.781909	-1.035095
6	-6.766762	-0.587093	-0.251481
6	-7.151313	0.313878	-1.230800
1	-8.193304	0.600939	-1.311334
6	-4.874424	0.536891	-2.058835
6	-6.219138	0.869590	-2.119571
1	-6.554037	1.577295	-2.868439
1	-7.482282	-1.011111	0.442600
1	-4.162328	0.979916	-2.741317
16	-2.080820	-2.415678	1.013412
7	-3.273520	-0.914623	-0.694647
7	-4.790612	-1.778127	0.742309
6	-1.598844	-0.034874	-2.280976
1	-1.732811	1.040563	-2.144339
1	-0.579425	-0.227727	-2.602651
1	-2.266481	-0.364379	-3.080391
6	3.560890	-1.408441	-0.506000
6	4.574901	-1.145422	-1.443171
6	5.765073	-1.849492	-1.465683
6	5.943817	-2.845174	-0.506243
6	4.961405	-3.106677	0.444556
6	3.767409	-2.386705	0.457216
6	2.491122	-0.426122	-0.743968
6	2.935211	0.378032	-1.923335

1	6.530813	-1.631974	-2.200528
1	6.865387	-3.415841	-0.500134
1	5.126374	-3.878199	1.187643
1	3.000092	-2.579772	1.193222
7	4.176452	-0.090497	-2.266986
1	4.703543	0.273908	-3.044277
8	2.328914	1.269115	-2.500037
6	1.942980	3.002130	0.119273
7	1.991045	1.740493	0.871998
6	0.846956	1.060648	1.190421
6	3.159990	1.096407	0.819905
6	-0.521683	1.569712	1.086661
6	-1.276204	0.876654	2.049206
6	-2.650342	1.002636	2.143910
6	-3.285107	1.856430	1.245509
6	-2.558588	2.555309	0.285718
6	-1.176189	2.411476	0.193957
6	0.868117	0.136422	2.367167
1	-3.213772	0.441607	2.879137
1	-0.638026	2.939357	-0.582518
1	1.565953	2.804056	-0.883891
7	-0.432294	0.059340	2.792595
1	3.280849	0.241095	1.467224
8	1.817201	-0.433545	2.873410
1	-0.723340	-0.555014	3.535852
1	-4.362529	1.964590	1.287494
6	4.333361	1.936529	0.443937
1	4.872419	1.512967	-0.405682
1	-3.073671	3.206441	-0.409948
16	3.660633	3.592541	0.054406
1	5.025779	2.019316	1.282196
1	1.319636	3.720093	0.647543

TS-CC-mx

E(RwB97XD) = -2490.84077694 A.U.

Imaginary frequency = -336.6023 cm⁻¹

6	1.006587	-0.985953	0.063196
1	0.468370	-1.583867	-0.656935
6	0.239853	-0.405815	1.151001
8	0.724875	0.267401	2.057978
6	-4.683355	-1.116828	0.103019
6	-5.523649	-0.272668	0.861802
6	-3.571803	0.108204	1.575895
6	-1.233704	-0.537524	1.124544

6	-2.101680	-1.251453	0.356407
6	-6.897696	-0.269642	0.619671
6	-7.390244	-1.099953	-0.373550
1	-8.454416	-1.112693	-0.578639
6	-5.170628	-1.942835	-0.904713
6	-6.539453	-1.921891	-1.126750
1	-6.957076	-2.552618	-1.902369
1	-7.550293	0.373641	1.197506
1	-4.524378	-2.571620	-1.501509
16	-2.048662	0.562034	2.252503
7	-3.407783	-0.854032	0.598240
7	-4.800664	0.482600	1.777627
6	-1.876206	-2.381173	-0.592494
1	-1.948575	-2.052171	-1.632057
1	-0.909895	-2.851217	-0.436373
1	-2.637424	-3.144423	-0.422191
6	3.467427	-0.920967	0.995460
6	4.489516	-1.853768	0.749254
6	5.679982	-1.862528	1.454829
6	5.850585	-0.898914	2.445657
6	4.852480	0.033249	2.711623
6	3.659568	0.028082	1.991971
6	2.394592	-1.185124	0.010852
6	2.849477	-2.409313	-0.748506
1	6.449628	-2.594303	1.241748
1	6.772467	-0.880587	3.015353
1	5.000447	0.772368	3.489983
1	2.873505	0.731788	2.221683
7	4.103326	-2.705196	-0.284988
1	4.639833	-3.487422	-0.624421
8	2.248408	-3.019306	-1.611492
6	2.807523	2.237924	-0.597044
7	2.121192	1.156004	-1.312386
6	0.769307	1.020479	-1.248381
6	2.901917	0.112802	-1.656261
6	-0.178807	1.978253	-0.685477
6	-1.423963	1.700945	-1.281012
6	-2.580172	2.372455	-0.933943
6	-2.479917	3.375027	0.028239
6	-1.262302	3.666705	0.633453
6	-0.110219	2.959894	0.299305
6	0.035512	0.275111	-2.319160
1	-3.527929	2.129343	-1.398840
1	0.813039	3.183983	0.814025
1	2.689293	2.100412	0.477061
7	-1.270660	0.680964	-2.213647

1	2.468434	-0.588860	-2.356604
8	0.462979	-0.515790	-3.140361
1	-1.983684	0.370188	-2.854002
1	-3.368964	3.923711	0.315559
6	4.360939	0.428263	-1.730496
1	4.956651	-0.273433	-1.145389
1	-1.209316	4.438769	1.391101
16	4.553911	2.125992	-1.080975
1	4.703393	0.397574	-2.764973
1	2.396116	3.195940	-0.907412

TS-CO-on

$E(\text{RwB97XD}) = -2490.83341750 \text{ A.U.}$

Imaginary frequency = $-388.8288 \text{ cm}^{-1}$

6	-1.378551	-0.934807	-1.030165
1	-0.814460	-1.858084	-1.028377
6	-0.651779	0.281987	-0.800645
8	-1.273683	1.408922	-0.635644
6	4.380132	-0.222784	-1.244760
6	5.048948	1.015982	-1.357551
6	2.997013	1.500229	-1.256104
6	0.790204	0.398777	-0.978441
6	1.810174	-0.506984	-0.999988
6	6.441069	1.045245	-1.443899
6	7.124079	-0.159090	-1.414686
1	8.205957	-0.160550	-1.479036
6	5.061225	-1.436240	-1.222544
6	6.444020	-1.381257	-1.306590
1	7.009441	-2.305344	-1.290903
1	6.961254	1.991495	-1.530789
1	4.550267	-2.386034	-1.148659
16	1.365904	2.076753	-1.149061
7	3.033818	0.125802	-1.186119
7	4.154473	2.080944	-1.361507
6	1.815212	-1.987352	-0.862941
1	2.554299	-2.277043	-0.112221
1	0.859150	-2.375964	-0.532637
1	2.081389	-2.458808	-1.813073
6	-3.898321	-0.278423	-1.327047
6	-5.012393	-1.140010	-1.296957
6	-6.307721	-0.681133	-1.452056
6	-6.490935	0.684142	-1.664944
6	-5.403556	1.550310	-1.736889
6	-4.104287	1.074748	-1.576212

6	-2.713816	-1.117185	-1.147632
6	-3.214524	-2.531285	-1.063847
1	-7.149532	-1.362097	-1.417500
1	-7.496067	1.070738	-1.788048
1	-5.566536	2.605104	-1.923347
1	-3.259887	1.745733	-1.645860
7	-4.582179	-2.452919	-1.124683
1	-5.182722	-3.260114	-1.085984
8	-2.561747	-3.551192	-0.943686
6	-0.135823	2.301173	2.172053
7	-1.036639	1.214146	1.790915
6	-0.617304	-0.101810	1.790885
6	-2.030625	1.571826	0.950562
6	0.679427	-0.634991	2.098384
6	0.501304	-2.029089	2.278150
6	1.561162	-2.882830	2.516604
6	2.843434	-2.336368	2.554101
6	3.049543	-0.973096	2.349349
6	1.978163	-0.117970	2.112596
6	-1.590060	-1.197878	1.892032
1	1.399724	-3.945446	2.651406
1	2.169444	0.934681	1.950442
1	0.696197	2.371588	1.472016
7	-0.840432	-2.331765	2.133746
1	-2.811135	0.834638	0.816727
8	-2.809129	-1.168545	1.776762
1	-1.247965	-3.249356	2.205266
1	3.691695	-2.985620	2.736515
6	-2.406790	3.016152	1.034082
1	-2.422181	3.454587	0.037466
1	4.055871	-0.572407	2.364421
16	-1.146018	3.811737	2.095933
1	-3.388680	3.126753	1.491833
1	0.227721	2.138848	3.185066

TS-CO-ox

E(RwB97XD) = -2490.83120591 A.U.

Imaginary frequency = -397.5229 cm⁻¹

6	0.712817	0.506460	-1.253685
1	0.128359	1.402786	-1.427985
6	-0.005277	-0.616576	-0.736982
8	0.561435	-1.757903	-0.514780
6	-4.988536	0.341118	-0.572940
6	-5.780574	-0.825832	-0.648208

6	-3.783754	-1.505230	-0.730572
6	-1.468566	-0.617354	-0.694071
6	-2.391781	0.375506	-0.579774
6	-7.171598	-0.718624	-0.624027
6	-7.729214	0.545492	-0.530163
1	-8.807548	0.652382	-0.510092
6	-5.543524	1.614313	-0.487379
6	-6.927363	1.694826	-0.464761
1	-7.397369	2.668735	-0.398082
1	-7.787144	-1.608286	-0.680308
1	-4.937002	2.508434	-0.446068
16	-2.213949	-2.230147	-0.815362
7	-3.681289	-0.134564	-0.627228
7	-4.997309	-1.970224	-0.746609
6	-2.219230	1.844746	-0.408217
1	-2.845652	2.193483	0.415126
1	-1.193176	2.108823	-0.173130
1	-2.521545	2.374646	-1.316131
6	3.210230	-0.179335	-1.621899
6	4.293880	0.663644	-1.948508
6	5.583464	0.186493	-2.088954
6	5.790861	-1.182662	-1.920907
6	4.733261	-2.039556	-1.632747
6	3.438668	-1.545457	-1.484802
6	2.025166	0.664805	-1.555519
6	2.475662	2.047942	-1.929493
1	6.402691	0.852744	-2.330955
1	6.792906	-1.582172	-2.026738
1	4.914626	-3.101582	-1.519184
1	2.613319	-2.207583	-1.263955
7	3.836414	1.967265	-2.104805
1	4.404755	2.755166	-2.368781
8	1.800015	3.051483	-2.053392
6	2.765281	-1.444513	1.773750
7	1.328428	-1.182174	1.729240
6	0.828423	0.100234	1.760415
6	0.581248	-2.180254	1.219788
6	1.557053	1.332236	1.712448
6	0.633778	2.349239	2.059429
6	0.958850	3.688526	2.003031
6	2.251012	4.030538	1.596660
6	3.176555	3.051630	1.253706
6	2.837746	1.701041	1.292591
6	-0.531335	0.387394	2.230638
1	0.232411	4.449887	2.260927
1	3.576977	0.963365	1.012020

1	3.198373	-0.960282	2.646828
7	-0.576186	1.759237	2.387261
1	-0.483594	-2.103704	1.399332
8	-1.464683	-0.376903	2.445682
1	-1.409607	2.247957	2.669218
1	2.530373	5.076245	1.545835
6	1.233719	-3.524578	1.271355
1	0.696974	-4.183149	1.952270
1	4.170148	3.338556	0.931288
16	2.926686	-3.249374	1.905639
1	1.242774	-3.968200	0.276448
1	3.248082	-1.093378	0.861387

TS-CO-mn

$E(\text{RwB97XD}) = -2490.81610435 \text{ A.U.}$

Imaginary frequency = $-360.8181 \text{ cm}^{-1}$

6	-0.862090	-1.929941	0.420976
1	-0.258817	-2.544098	1.080494
6	-0.314175	-0.593000	0.077524
8	-1.028666	0.257084	-0.543108
6	4.761230	-0.915915	-0.639507
6	5.270016	0.186242	-1.364347
6	3.189348	0.515388	-1.231928
6	1.151565	-0.517683	-0.266344
6	2.252175	-1.269782	-0.026998
6	6.639685	0.270638	-1.621965
6	7.459615	-0.740708	-1.151337
1	8.525915	-0.695117	-1.340562
6	5.582912	-1.933879	-0.162616
6	6.938579	-1.826890	-0.431690
1	7.608681	-2.600987	-0.076910
1	7.037412	1.111903	-2.176972
1	5.196330	-2.776269	0.394073
16	1.507104	0.929814	-1.237753
7	3.393665	-0.671119	-0.571652
7	4.261399	1.069047	-1.724587
6	2.449327	-2.574529	0.670463
1	3.115257	-2.451639	1.529289
1	1.519736	-3.010457	1.018447
1	2.911422	-3.291315	-0.013457
6	-3.197870	-2.115961	-0.729819
6	-4.094440	-3.197876	-0.662930
6	-5.314459	-3.191403	-1.313484
6	-5.644314	-2.057859	-2.055668

6	-4.773553	-0.975397	-2.136136
6	-3.546573	-0.996747	-1.474901
6	-2.031536	-2.483883	0.079927
6	-2.323788	-3.862037	0.624141
1	-5.988872	-4.036596	-1.247409
1	-6.595248	-2.024383	-2.575226
1	-5.050990	-0.104104	-2.717922
1	-2.864469	-0.160385	-1.520948
7	-3.554413	-4.208222	0.134809
1	-4.003744	-5.085169	0.342565
8	-1.624424	-4.543043	1.348862
6	0.777370	2.217480	1.939112
7	-0.455376	1.435804	1.747853
6	-1.469591	1.921342	1.050083
6	-0.364723	0.092259	2.027798
6	-1.593474	3.179165	0.334767
6	-2.907005	3.201269	-0.176078
6	-3.369050	4.226394	-0.979721
6	-2.491555	5.267224	-1.270449
6	-1.192706	5.274757	-0.768688
6	-0.733980	4.234629	0.031999
6	-2.829613	1.274332	1.050634
1	-4.380964	4.218733	-1.364885
1	0.276826	4.276016	0.410599
1	1.158864	2.540570	0.973832
7	-3.600379	2.078583	0.256119
1	-1.314910	-0.369080	2.259697
8	-3.215625	0.297098	1.657156
1	-4.569395	1.881367	0.065605
1	-2.829972	6.086065	-1.894269
6	0.794362	-0.239416	2.914270
1	1.265640	-1.177557	2.622875
1	-0.529405	6.098352	-1.001258
16	1.999523	1.114672	2.710229
1	0.483422	-0.318066	3.957198
1	0.546582	3.073392	2.571905

TS-CO-mx

E(RwB97XD) = -2490.81994493 A.U.

Imaginary frequency = -359.7853 cm⁻¹

6	0.217166	1.380738	0.067848
1	-0.332895	2.020536	0.750708
6	-0.291927	0.001894	-0.139206
8	0.429977	-0.841037	-0.760610

6	-5.392086	0.330318	-0.511532
6	-6.007289	-0.918570	-0.757123
6	-3.937530	-1.321951	-0.665862
6	-1.780558	-0.159266	-0.296140
6	-2.821460	0.706669	-0.275361
6	-7.397256	-0.994408	-0.864058
6	-8.131156	0.170707	-0.719249
1	-9.211539	0.134296	-0.798637
6	-6.126841	1.502515	-0.355554
6	-7.505042	1.400751	-0.466386
1	-8.110005	2.292445	-0.352164
1	-7.876772	-1.947443	-1.053040
1	-5.658317	2.455434	-0.151318
16	-2.281469	-1.830739	-0.634720
7	-4.034419	0.032430	-0.461696
7	-5.070303	-1.939090	-0.849303
6	-2.877213	2.194903	-0.163150
1	-1.897338	2.649052	-0.266298
1	-3.506407	2.591412	-0.963309
1	-3.309161	2.504157	0.792767
6	2.472254	1.510757	-1.254821
6	3.414557	2.554971	-1.220108
6	4.607628	2.503510	-1.916847
6	4.856329	1.368119	-2.686248
6	3.933327	0.329531	-2.749160
6	2.740843	0.390583	-2.033805
6	1.358459	1.919528	-0.390038
6	1.705932	3.307472	0.100288
1	5.319363	3.318949	-1.868832
1	5.784519	1.298920	-3.242165
1	4.150614	-0.547160	-3.347304
1	2.026552	-0.418491	-2.054632
7	2.944247	3.589307	-0.407922
1	3.415074	4.466485	-0.256007
8	1.039980	4.035748	0.809910
6	1.880163	0.334605	2.567318
7	1.213014	-0.760836	1.850586
6	1.888382	-1.580650	1.063448
6	-0.161044	-0.652142	1.759391
6	3.269728	-1.516610	0.639606
6	3.468092	-2.639752	-0.187931
6	4.661794	-2.864259	-0.847968
6	5.686401	-1.940768	-0.663107
6	5.515572	-0.824850	0.152364
6	4.309301	-0.599518	0.800790
6	1.322984	-2.884375	0.565703

1	4.792251	-3.729700	-1.485615
1	4.205180	0.279642	1.419533
1	2.309349	1.031443	1.849050
7	2.315834	-3.414987	-0.215217
1	-0.653267	-1.592434	1.550467
8	0.273979	-3.424774	0.849115
1	2.230566	-4.313625	-0.661452
1	6.633277	-2.094901	-1.167151
6	-0.758600	0.188464	2.844814
1	-1.531950	0.849029	2.448077
1	6.325611	-0.117114	0.274325
16	0.605652	1.173541	3.557441
1	-1.202624	-0.432178	3.623503
1	2.655422	-0.084355	3.206008

9a

E(RwB97XD) = -2490.89736427 A.U.

6	0.827010	1.527094	0.292324
1	0.566293	1.947261	-0.680700
6	-0.324907	1.724681	1.259418
8	-0.132171	2.138669	2.385474
6	-4.629788	0.156055	-0.939057
6	-5.566464	-0.349253	-0.011932
6	-3.926177	0.286756	1.156944
6	-1.675966	1.269050	0.882589
6	-2.310238	1.138067	-0.314970
6	-6.779274	-0.865300	-0.468371
6	-7.018458	-0.864492	-1.832672
1	-7.954130	-1.260490	-2.209837
6	-4.860401	0.152678	-2.310636
6	-6.073210	-0.364707	-2.740171
1	-6.291687	-0.383497	-3.801121
1	-7.504639	-1.254880	0.235488
1	-4.136925	0.529433	-3.020386
16	-2.678809	0.761329	2.257420
7	-3.560632	0.568423	-0.145709
7	-5.098179	-0.253584	1.294957
6	-1.935146	1.589132	-1.684591
1	-2.745233	2.205923	-2.081056
1	-1.031347	2.188200	-1.689162
1	-1.791350	0.738856	-2.354476
6	0.489205	-1.018382	0.936940
6	-0.179609	-1.926831	0.113998
6	-0.908026	-2.990823	0.610479

6	-0.965869	-3.137930	1.995209
6	-0.323733	-2.237037	2.835451
6	0.402887	-1.168009	2.311713
6	1.169414	0.020809	0.062782
6	0.678232	-0.393106	-1.346150
1	-1.420796	-3.677161	-0.052016
1	-1.529823	-3.961379	2.417432
1	-0.394829	-2.356279	3.909664
1	0.886420	-0.463882	2.974121
7	-0.023184	-1.546954	-1.221240
1	-0.457803	-2.002617	-2.008590
8	0.847182	0.221628	-2.380082
6	3.359625	1.955150	-1.292396
7	3.202201	1.418541	0.061653
6	2.782693	0.021591	0.145254
6	2.148473	2.167325	0.759584
6	3.469853	-0.980925	-0.768267
6	4.071649	-1.963869	0.021845
6	4.744429	-3.046759	-0.513159
6	4.825961	-3.132941	-1.900802
6	4.249381	-2.161407	-2.709382
6	3.565408	-1.082960	-2.148238
6	3.253067	-0.479127	1.553466
1	5.197743	-3.794219	0.126251
1	3.107026	-0.349182	-2.794901
1	2.575910	1.628069	-1.979169
7	3.898029	-1.659888	1.371938
1	2.251998	2.000081	1.828614
8	3.110105	0.084340	2.615616
1	4.335620	-2.153301	2.134361
1	5.349897	-3.968079	-2.350857
6	2.301985	3.651100	0.446239
1	1.333532	4.136349	0.325771
1	4.326940	-2.238924	-3.786917
16	3.268387	3.765031	-1.107604
1	2.855486	4.160317	1.232481
1	4.337858	1.691011	-1.691950

11a

E(RwB97XD) = -2490.88333459 A.U.

6	-0.686184	1.313405	0.975877
1	-0.191609	1.275315	1.944729
6	0.307736	1.806905	-0.059346
8	-0.047092	2.540322	-0.966309

6	4.916988	-0.269847	0.534330
6	5.773402	0.010690	-0.551620
6	3.966702	1.005633	-1.010805
6	1.708150	1.360314	-0.066965
6	2.479275	0.591814	0.755237
6	7.066297	-0.511003	-0.565884
6	7.465822	-1.298225	0.501615
1	8.466362	-1.714490	0.512138
6	5.310561	-1.063573	1.606463
6	6.600916	-1.571175	1.570504
1	6.944284	-2.193435	2.388147
1	7.729209	-0.299703	-1.396052
1	4.654138	-1.287278	2.435557
16	2.566525	1.871553	-1.540220
7	3.735004	0.398461	0.210617
7	5.150521	0.812610	-1.503974
6	2.215317	-0.026306	2.082607
1	2.992004	0.285982	2.784333
1	1.257827	0.253574	2.502658
1	2.250044	-1.116068	1.998974
6	-0.651724	-0.811596	-0.605191
6	-0.269337	-2.106627	-0.249076
6	0.233615	-3.018095	-1.158265
6	0.371132	-2.600887	-2.479897
6	0.015736	-1.312166	-2.857938
6	-0.501413	-0.416111	-1.923960
6	-1.205356	-0.118127	0.627742
6	-0.840126	-1.137384	1.737396
1	0.518392	-4.016298	-0.849457
1	0.766693	-3.290209	-3.216497
1	0.137152	-0.996636	-3.886844
1	-0.767598	0.582059	-2.244389
7	-0.450504	-2.288047	1.124409
1	-0.126883	-3.088293	1.645559
8	-0.876852	-0.946456	2.932525
6	-3.136439	2.060433	-0.934999
7	-3.048990	1.505631	0.407079
6	-2.830373	0.086667	0.575284
6	-1.987166	2.168463	1.162366
6	-3.522570	-0.885414	-0.356202
6	-4.162972	-1.857261	0.416519
6	-4.816284	-2.940872	-0.141580
6	-4.839847	-3.034072	-1.531144
6	-4.231781	-2.066419	-2.321986
6	-3.566101	-0.990285	-1.736835
6	-3.477779	-0.312346	1.951029

1	-5.300856	-3.682396	0.481633
1	-3.093218	-0.254192	-2.370732
1	-4.089352	1.804146	-1.396094
7	-4.051280	-1.539492	1.772819
1	-2.235031	2.059398	2.216574
8	-3.516124	0.339590	2.964816
1	-4.603087	-1.970563	2.498397
1	-5.347158	-3.870264	-1.998003
6	-1.992706	3.660351	0.806698
1	-2.435655	4.237659	1.615918
1	-4.269778	-2.146597	-3.401345
16	-3.069685	3.854382	-0.666389
1	-0.999162	4.044908	0.595588
1	-2.309846	1.775318	-1.591816

12a

E(RwB97XD) = -2490.89712032 A.U.

6	1.127592	-0.060287	-0.115834
1	0.630970	0.390406	-0.972413
6	0.412303	-1.346515	0.250634
8	0.933141	-2.224159	0.907656
6	-4.395156	-0.515313	-1.098846
6	-5.320649	-1.000797	-0.150898
6	-3.434041	-1.651277	0.540956
6	-1.039675	-1.397026	-0.001130
6	-1.827161	-0.815931	-0.945442
6	-6.678349	-0.722439	-0.307561
6	-7.068486	0.035222	-1.399557
1	-8.118120	0.265056	-1.540900
6	-4.778790	0.251174	-2.193699
6	-6.133283	0.516095	-2.327654
1	-6.473672	1.109198	-3.167926
1	-7.397051	-1.090969	0.414225
1	-4.066199	0.630251	-2.913125
16	-1.970901	-2.235047	1.258848
7	-3.164177	-0.961265	-0.626023
7	-4.688933	-1.711964	0.865387
6	-1.475331	-0.172341	-2.242133
1	-1.764097	0.881031	-2.245895
1	-0.415944	-0.250048	-2.470107
1	-2.023003	-0.676184	-3.042618
6	3.519086	-1.274278	-0.240253
6	4.131310	-1.606506	-1.447674
6	5.066367	-2.621036	-1.553985

6	5.393986	-3.312597	-0.389565
6	4.810433	-2.980956	0.829889
6	3.873072	-1.952179	0.912728
6	2.636342	-0.067004	-0.456660
6	2.757797	0.141672	-1.986053
1	5.528944	-2.862495	-2.503275
1	6.120436	-4.115673	-0.437665
1	5.085592	-3.528360	1.723608
1	3.410322	-1.690094	1.855415
7	3.665382	-0.752801	-2.455188
1	3.904514	-0.820971	-3.431976
8	2.134285	0.940309	-2.658247
6	1.813127	3.010440	-0.220348
7	2.049313	1.976397	0.785763
6	0.954055	1.046920	1.015310
6	3.192047	1.154999	0.390621
6	-0.461876	1.579596	1.052402
6	-1.073615	1.121052	2.219265
6	-2.424359	1.291725	2.464276
6	-3.175126	1.960005	1.499958
6	-2.582050	2.443393	0.338699
6	-1.220943	2.248268	0.107095
6	1.099562	0.424961	2.436224
1	-2.883292	0.903449	3.364844
1	-0.781158	2.603698	-0.816058
1	1.370906	2.624113	-1.143410
7	-0.136631	0.448649	3.007665
1	3.600771	0.704344	1.292447
8	2.108815	-0.004092	2.948342
1	-0.312666	0.088692	3.932817
1	-4.238160	2.098288	1.658051
6	4.252457	2.041555	-0.270056
1	4.634601	1.608201	-1.194176
1	-3.182316	2.960329	-0.399912
16	3.463864	3.662239	-0.599165
1	5.091262	2.207496	0.402422
1	1.201480	3.812009	0.191222

13a

E(RwB97XD) = -2490.90190788 A.U.

6	1.023786	-0.226666	-0.736599
1	0.623744	-0.056620	-1.738792
6	0.284520	-1.403908	-0.128217
8	0.845903	-2.327872	0.416329

6	-4.634741	-0.378082	-0.828538
6	-5.441560	-0.748973	0.268700
6	-3.492170	-1.378926	0.781983
6	-1.191003	-1.311393	-0.104269
6	-2.076569	-0.780534	-0.989086
6	-6.806074	-0.459443	0.249332
6	-7.320467	0.192555	-0.859122
1	-8.377841	0.427437	-0.895773
6	-5.142776	0.284909	-1.940538
6	-6.501620	0.560912	-1.936860
1	-6.937484	1.074393	-2.785416
1	-7.434497	-0.740057	1.085823
1	-4.518725	0.580136	-2.772830
16	-1.965219	-1.958052	1.354253
7	-3.359281	-0.804704	-0.467595
7	-4.697699	-1.375393	1.263871
6	-1.894940	-0.325086	-2.397794
1	-2.054595	0.750506	-2.498215
1	-0.908497	-0.571379	-2.780422
1	-2.625835	-0.840876	-3.025158
6	3.411675	-1.095222	0.026252
6	4.032744	-2.150851	-0.641942
6	4.919473	-3.004531	-0.012977
6	5.199843	-2.764254	1.332272
6	4.625450	-1.690214	2.002718
6	3.732122	-0.842423	1.345990
6	2.551867	-0.350179	-0.962580
6	2.786383	-1.128884	-2.270240
1	5.386242	-3.823269	-0.546945
1	5.889433	-3.417810	1.853842
1	4.876643	-1.504858	3.040187
1	3.313865	0.020239	1.847650
7	3.634069	-2.153636	-1.984828
1	3.943113	-2.816173	-2.678650
8	2.280942	-0.880066	-3.344913
6	2.362561	3.086548	0.222920
7	2.144691	1.670128	0.062955
6	0.799780	1.125965	0.040096
6	2.890585	1.151964	-1.075039
6	0.123966	1.065862	1.391112
6	-1.088809	1.751394	1.319818
6	-1.953158	1.836709	2.394465
6	-1.560420	1.221582	3.582780
6	-0.349766	0.544980	3.677112
6	0.500182	0.459459	2.573949
6	-0.201572	2.001936	-0.775840

1	-2.896335	2.363187	2.317276
1	1.428384	-0.092122	2.643475
1	2.130259	3.404518	1.239658
7	-1.253296	2.288368	0.036015
1	2.496460	1.522552	-2.032812
8	-0.056606	2.353649	-1.927377
1	-2.027235	2.867532	-0.251518
1	-2.215753	1.271808	4.444375
6	4.321745	1.635201	-0.897299
1	4.896258	0.983110	-0.242817
1	-0.067632	0.071737	4.609575
16	4.161312	3.287035	-0.099347
1	4.830436	1.745490	-1.853090
1	1.804590	3.695330	-0.498499

14a

E(RwB97XD) = -2490.86458368 A.U.

6	1.554282	-0.107125	-1.203349
1	1.336355	0.311442	-2.182805
6	0.867251	0.535152	-0.020750
8	1.659768	0.486139	1.146946
6	-3.679110	-1.777546	-0.076528
6	-4.103331	-2.248187	1.186478
6	-2.208241	-1.382278	1.519764
6	-0.405384	-0.223838	0.287388
6	-1.421443	-0.566232	-0.531051
6	-5.342542	-2.880887	1.304541
6	-6.116019	-3.023474	0.165320
1	-7.081329	-3.511534	0.234150
6	-4.452131	-1.918662	-1.225267
6	-5.677678	-2.549511	-1.081301
1	-6.309795	-2.679083	-1.951726
1	-5.678101	-3.245724	2.267880
1	-4.122404	-1.557570	-2.189968
16	-0.670071	-0.715289	1.970340
7	-2.432521	-1.218250	0.174129
7	-3.159342	-1.987290	2.171501
6	-1.615513	-0.305407	-1.984308
1	-2.522945	0.286176	-2.136523
1	-0.783565	0.250282	-2.406705
1	-1.712917	-1.244650	-2.534461
6	2.936483	-2.112566	-0.268959
6	3.706280	-3.027056	-1.010306
6	4.372889	-4.084564	-0.419853

6	4.256119	-4.230213	0.961533
6	3.494949	-3.342203	1.714981
6	2.831456	-2.278697	1.105802
6	2.373412	-1.158949	-1.233703
6	2.883598	-1.592365	-2.590829
1	4.961746	-4.775588	-1.010708
1	4.767675	-5.050504	1.451827
1	3.417565	-3.475227	2.787384
1	2.253462	-1.582603	1.694995
7	3.664430	-2.692010	-2.364851
1	4.133765	-3.195057	-3.100316
8	2.654211	-1.081064	-3.667623
6	0.307733	2.913836	2.093975
7	1.227433	2.726382	0.967948
6	0.652903	2.133228	-0.241158
6	2.253950	1.782224	1.350964
6	-0.733405	2.578115	-0.640117
6	-0.665386	3.162313	-1.906050
6	-1.786783	3.609455	-2.580141
6	-3.018498	3.464939	-1.946416
6	-3.111466	2.892848	-0.682220
6	-1.968121	2.443244	-0.024420
6	1.516331	2.656670	-1.433633
1	-1.707809	4.052564	-3.564969
1	-2.064105	1.985116	0.951199
1	-0.362962	2.065384	2.250202
7	0.659366	3.183156	-2.349121
1	3.111143	1.874487	0.684691
8	2.721575	2.614433	-1.526028
1	0.976931	3.617933	-3.201530
1	-3.916036	3.804008	-2.450112
6	2.624318	1.950524	2.814464
1	2.607291	0.980521	3.309285
1	-4.077751	2.787833	-0.204916
16	1.387253	3.088145	3.539901
1	3.611329	2.394586	2.921653
1	-0.273864	3.824792	1.964906

15a

E(RwB97XD) = -2490.86471681 A.U.

6	-0.891661	-0.246181	0.981341
1	-0.363587	0.279500	1.772774
6	-0.335545	0.021396	-0.385542
8	-1.036237	-0.681657	-1.388261

6	4.645608	-0.824763	0.408608
6	5.179881	-1.866440	-0.383271
6	3.142314	-1.744782	-0.918448
6	1.112093	-0.446015	-0.385236
6	2.165646	-0.032052	0.348255
6	6.530749	-2.199342	-0.262680
6	7.303282	-1.487151	0.638627
1	8.354157	-1.729089	0.747983
6	5.417791	-0.105661	1.316470
6	6.755142	-0.455380	1.416937
1	7.389722	0.080783	2.112560
1	6.950728	-2.996158	-0.864787
1	5.005623	0.690570	1.921357
16	1.499614	-1.782372	-1.476228
7	3.308680	-0.770343	0.035318
7	4.213776	-2.427134	-1.207996
6	2.266078	1.043366	1.375547
1	2.993573	1.798122	1.065832
1	1.314144	1.545298	1.531597
1	2.589154	0.625175	2.332233
6	-2.947490	-1.877599	0.891516
6	-3.781951	-2.221298	1.970826
6	-4.881295	-3.046927	1.825872
6	-5.144931	-3.555574	0.555367
6	-4.319677	-3.251838	-0.522338
6	-3.216328	-2.417134	-0.358884
6	-1.904952	-0.992058	1.429786
6	-2.180870	-0.892762	2.917551
1	-5.510721	-3.292890	2.672319
1	-6.001081	-4.204732	0.412333
1	-4.531959	-3.669874	-1.499047
1	-2.560008	-2.197446	-1.185119
7	-3.313238	-1.624152	3.141399
1	-3.729898	-1.729610	4.052307
8	-1.550910	-0.270937	3.748623
6	-2.953768	1.464841	-1.291975
7	-1.587080	1.493956	-1.833434
6	-0.526161	1.568937	-0.822899
6	-1.328368	0.228386	-2.475722
6	-0.729860	2.597737	0.267662
6	0.264070	3.572025	0.150940
6	0.361908	4.642419	1.020242
6	-0.582020	4.731826	2.040520
6	-1.581478	3.775646	2.177012
6	-1.659401	2.702299	1.291133
6	0.735517	2.127811	-1.563532

1	1.146123	5.381081	0.911099
1	-2.438360	1.963437	1.420975
1	-3.304538	2.475222	-1.091932
7	1.107065	3.264787	-0.916710
1	-0.441988	0.300202	-3.104351
8	1.265441	1.668125	-2.548223
1	1.877350	3.835459	-1.228492
1	-0.530643	5.559354	2.738212
6	-2.544747	-0.224316	-3.256621
1	-2.422059	0.012557	-4.311335
1	-2.304663	3.858301	2.978568
16	-3.967835	0.722148	-2.602243
1	-2.695552	-1.296847	-3.149784
1	-3.042207	0.854639	-0.389291

16a

E(RwB97XD) = -2490.86101783 A.U.

6	-0.382226	1.425577	-1.558459
1	-0.532117	1.504056	-2.632028
6	-0.540895	0.046982	-0.954402
8	-1.481551	0.069974	0.126446
6	4.320192	-1.101939	0.094746
6	4.495114	-1.864481	1.271391
6	2.414967	-1.555325	1.108926
6	0.764375	-0.436558	-0.360545
6	2.022334	-0.294565	-0.827368
6	5.781431	-2.238166	1.665406
6	6.848786	-1.839005	0.879275
1	7.856116	-2.117150	1.166798
6	5.389871	-0.694408	-0.696981
6	6.656166	-1.077534	-0.284137
1	7.515434	-0.779947	-0.873295
1	5.926831	-2.823138	2.565626
1	5.252656	-0.103223	-1.592149
16	0.690230	-1.367569	1.147501
7	2.945344	-0.917576	0.014110
7	3.280453	-2.134412	1.889506
6	2.513667	0.359419	-2.073288
1	3.130961	-0.340979	-2.641348
1	1.691226	0.677199	-2.708564
1	3.118670	1.238523	-1.834968
6	0.235773	2.952287	0.439967
6	0.609068	4.307141	0.406883
6	0.975965	4.998501	1.546261

6	0.958438	4.303996	2.755596
6	0.575327	2.967546	2.813357
6	0.206154	2.284705	1.655778
6	-0.067412	2.563181	-0.939189
6	0.118694	3.808578	-1.773826
1	1.263119	6.041891	1.501111
1	1.241868	4.820990	3.665168
1	0.557536	2.452748	3.766385
1	-0.115620	1.254820	1.709878
7	0.533567	4.782276	-0.903885
1	0.739713	5.725620	-1.190246
8	-0.039305	3.933787	-2.970543
6	-2.029206	-2.880098	-0.837969
7	-2.349209	-1.527062	-1.289877
6	-2.696527	-0.549887	-0.288010
6	-1.219700	-0.932586	-2.011855
6	-3.511378	-1.016415	0.886618
6	-4.767020	-0.412992	0.821397
6	-5.740806	-0.650609	1.773720
6	-5.416914	-1.508743	2.824039
6	-4.158906	-2.093979	2.919283
6	-3.191507	-1.844375	1.946084
6	-3.651724	0.492219	-0.962875
1	-6.714040	-0.180012	1.712456
1	-2.208714	-2.291167	2.029319
1	-1.358446	-2.908919	0.025590
7	-4.831685	0.439788	-0.286516
1	-1.617767	-0.301382	-2.804711
8	-3.392511	1.191184	-1.915032
1	-5.621122	1.022188	-0.518723
1	-6.160638	-1.712307	3.585596
6	-0.351183	-2.045724	-2.612144
1	0.644253	-2.063921	-2.172648
1	-3.926530	-2.743551	3.753912
16	-1.202330	-3.626080	-2.263997
1	-0.258052	-1.936739	-3.690461
1	-2.939633	-3.434315	-0.615182

17a

E(RwB97XD) = -2490.86283481 A.U.

6	0.516611	0.628838	1.416388
1	0.654447	0.498262	2.487343
6	0.214686	-0.601408	0.591482
8	1.046680	-0.618786	-0.574058

6	-4.844171	-0.301132	0.007410
6	-5.319539	-0.894282	-1.183995
6	-3.227129	-1.165054	-1.220499
6	-1.217727	-0.642556	0.123312
6	-2.342278	-0.198115	0.724249
6	-6.687844	-0.881693	-1.461906
6	-7.536619	-0.280211	-0.548445
1	-8.602384	-0.258712	-0.744618
6	-5.693241	0.305160	0.928796
6	-7.046693	0.304662	0.629657
1	-7.739856	0.767198	1.322187
1	-7.062242	-1.333752	-2.372563
1	-5.327165	0.759709	1.839251
16	-1.529952	-1.458147	-1.422440
7	-3.468696	-0.495635	-0.045619
7	-4.282216	-1.428951	-1.936951
6	-2.546795	0.504753	2.023308
1	-1.612211	0.653898	2.555046
1	-2.998962	1.486014	1.856163
1	-3.215970	-0.077665	2.661621
6	0.559568	2.553752	-0.318896
6	0.824372	3.914843	-0.087333
6	0.793615	4.854335	-1.100527
6	0.480688	4.407201	-2.383674
6	0.209238	3.065489	-2.634035
6	0.247814	2.128938	-1.603248
6	0.667615	1.878064	0.975977
6	1.017207	2.953365	1.980767
1	1.002519	5.898767	-0.904681
1	0.449072	5.121856	-3.198034
1	-0.031770	2.743693	-3.639891
1	0.051919	1.085707	-1.804597
7	1.098386	4.118199	1.267857
1	1.311885	5.008182	1.688552
8	1.192740	2.821045	3.173996
6	2.860736	-1.282262	2.063029
7	2.100860	-1.958910	1.009643
6	2.199597	-1.429663	-0.340875
6	0.663549	-1.923554	1.285119
6	3.483028	-0.744550	-0.724372
6	4.160684	-1.558180	-1.631410
6	5.377448	-1.187370	-2.174095
6	5.896176	0.052059	-1.799816
6	5.208610	0.894109	-0.931582
6	3.984553	0.499623	-0.392430
6	2.183897	-2.667821	-1.295918

1	5.899154	-1.826276	-2.875869
1	3.433230	1.163354	0.263252
1	2.889504	-0.195205	1.961079
7	3.401286	-2.703136	-1.906734
1	0.186947	-2.738780	0.738729
8	1.278869	-3.457003	-1.427692
1	3.652870	-3.408545	-2.581274
1	6.847429	0.369693	-2.210755
6	0.424715	-2.077156	2.779153
1	-0.360340	-1.410051	3.136752
1	5.621115	1.862838	-0.678412
16	2.015179	-1.713695	3.617463
1	0.139699	-3.099157	3.016726
1	3.879612	-1.665664	2.094721