
Supporting Information

Structural factors controlling the spin-spin exchange coupling: EPR spectroscopic studies of strongly asymmetric trityl-nitroxide biradicals

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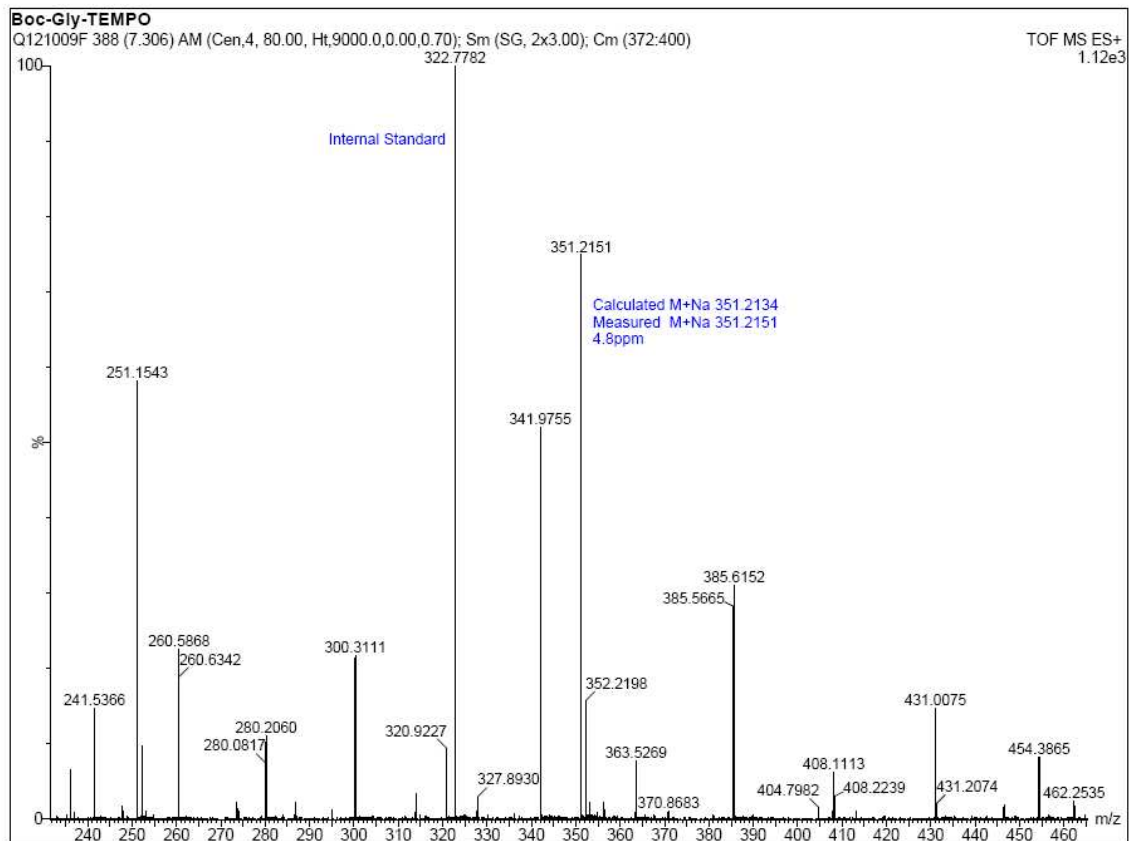


Figure S1. Mass spectrum (ESI) of GT.

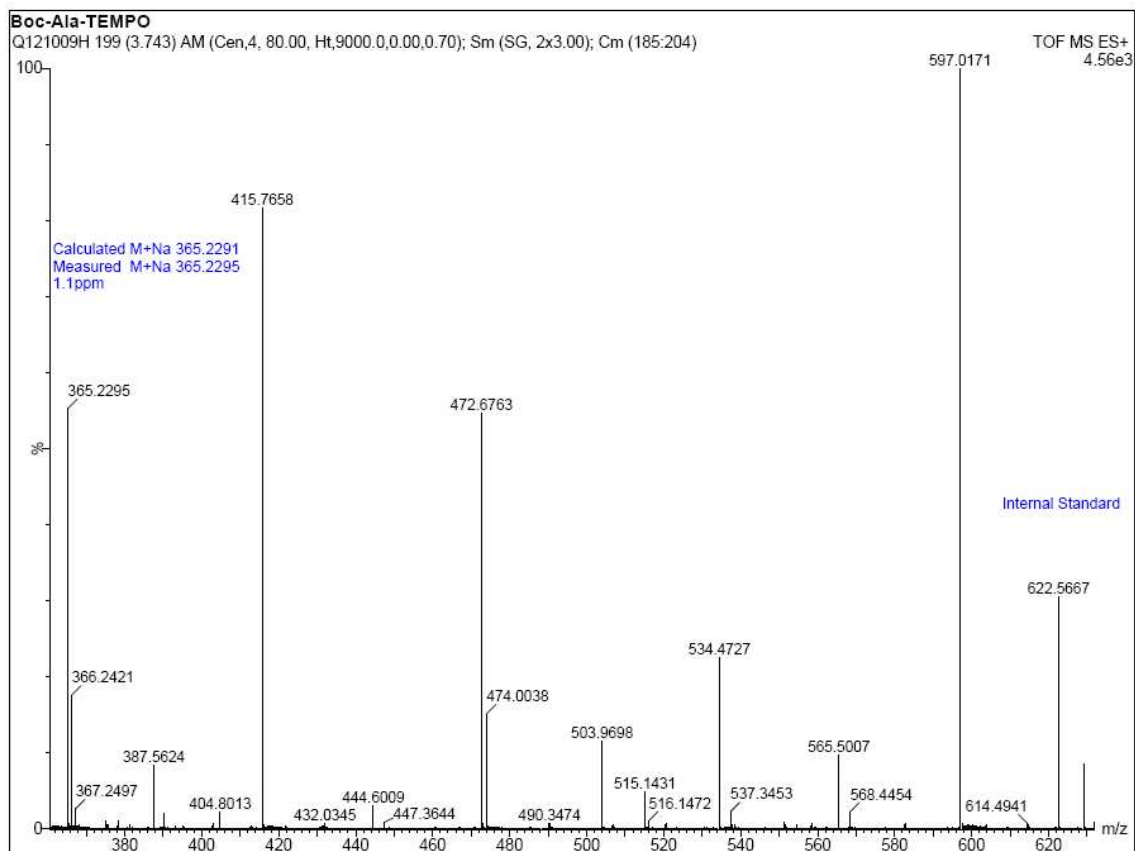


Figure S2. Mass spectrum (ESI) of AT.

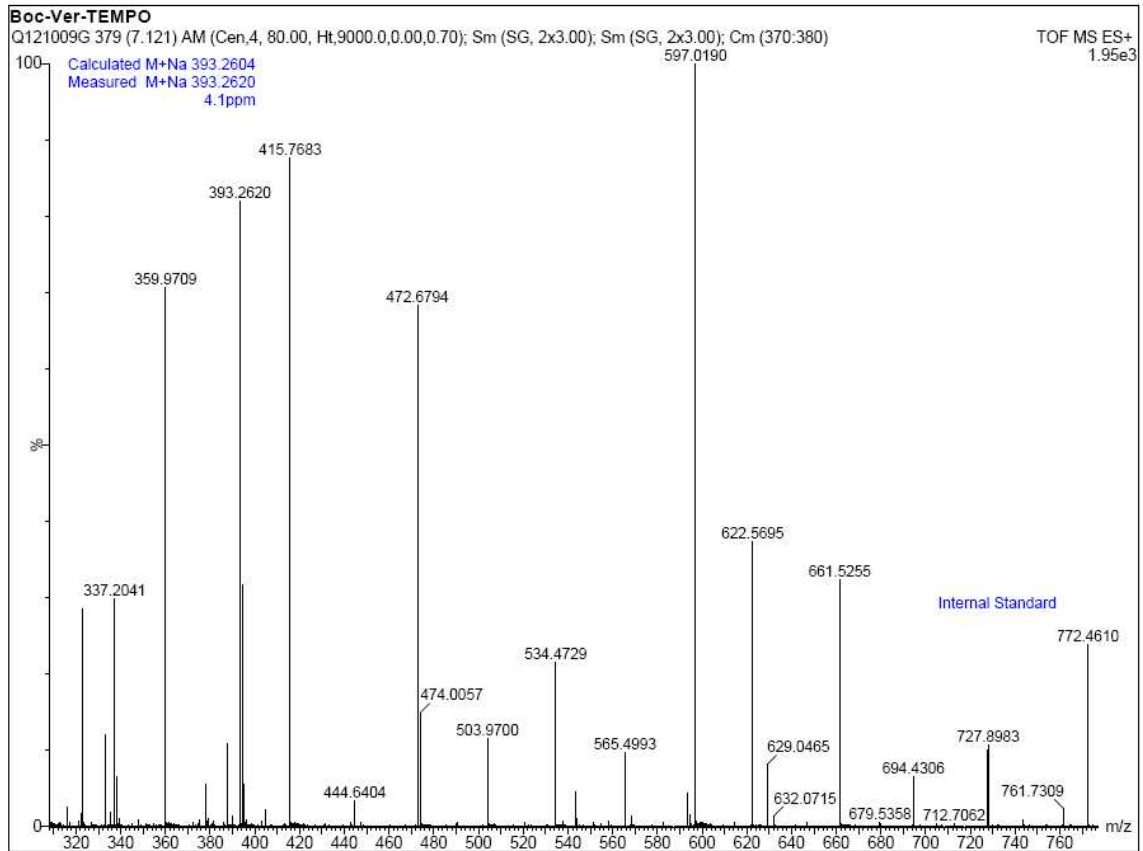


Figure S3. Mass spectrum (ESI) of VT.

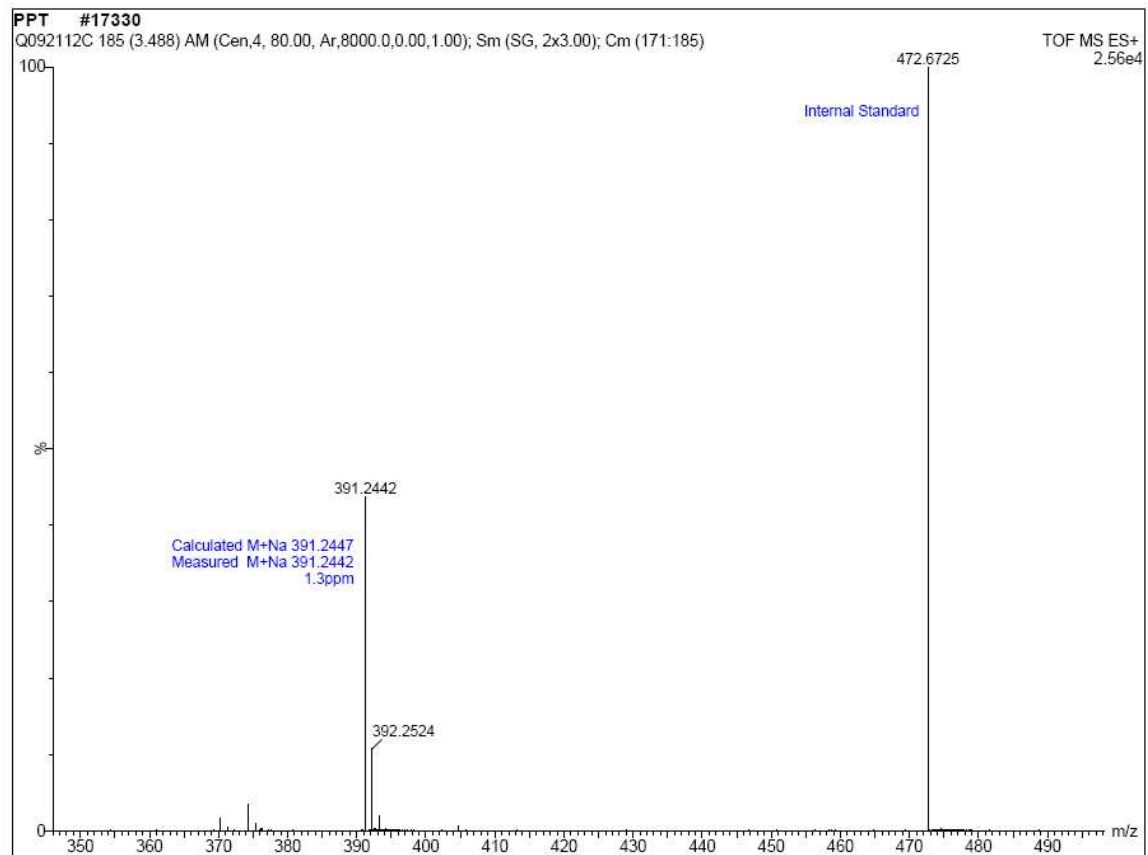


Figure S4. Mass spectrum (ESI) of PPT.

D:\DATA\MALDI\Dec 09\M121009\15149 CT02 GLY TEMPO\0_F4\1

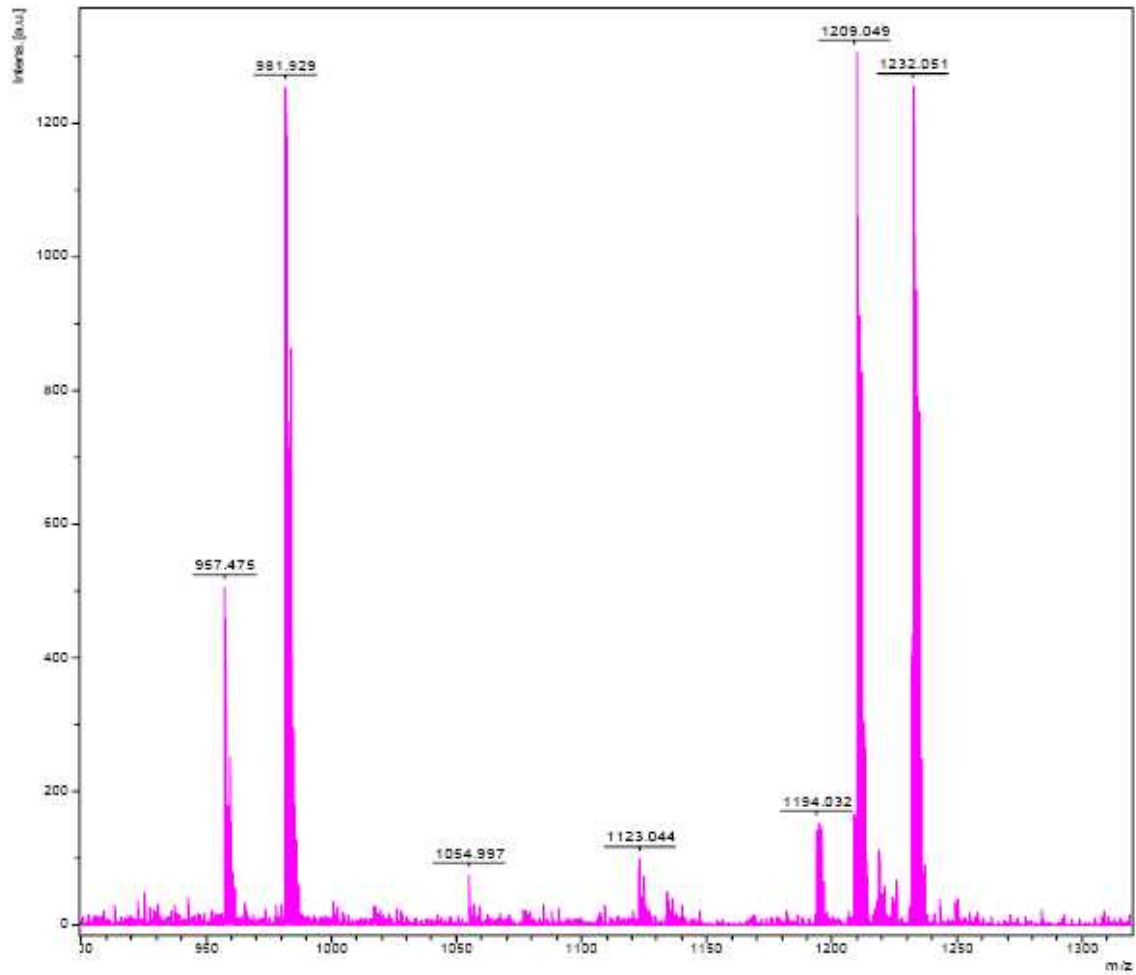


Figure S5. Mass spectrum (MALDI) of CT02-GT.

D:\DATA\MALDI\Dec 09\M121009\15149 CT02 ALA TEMPO\0_F5\1

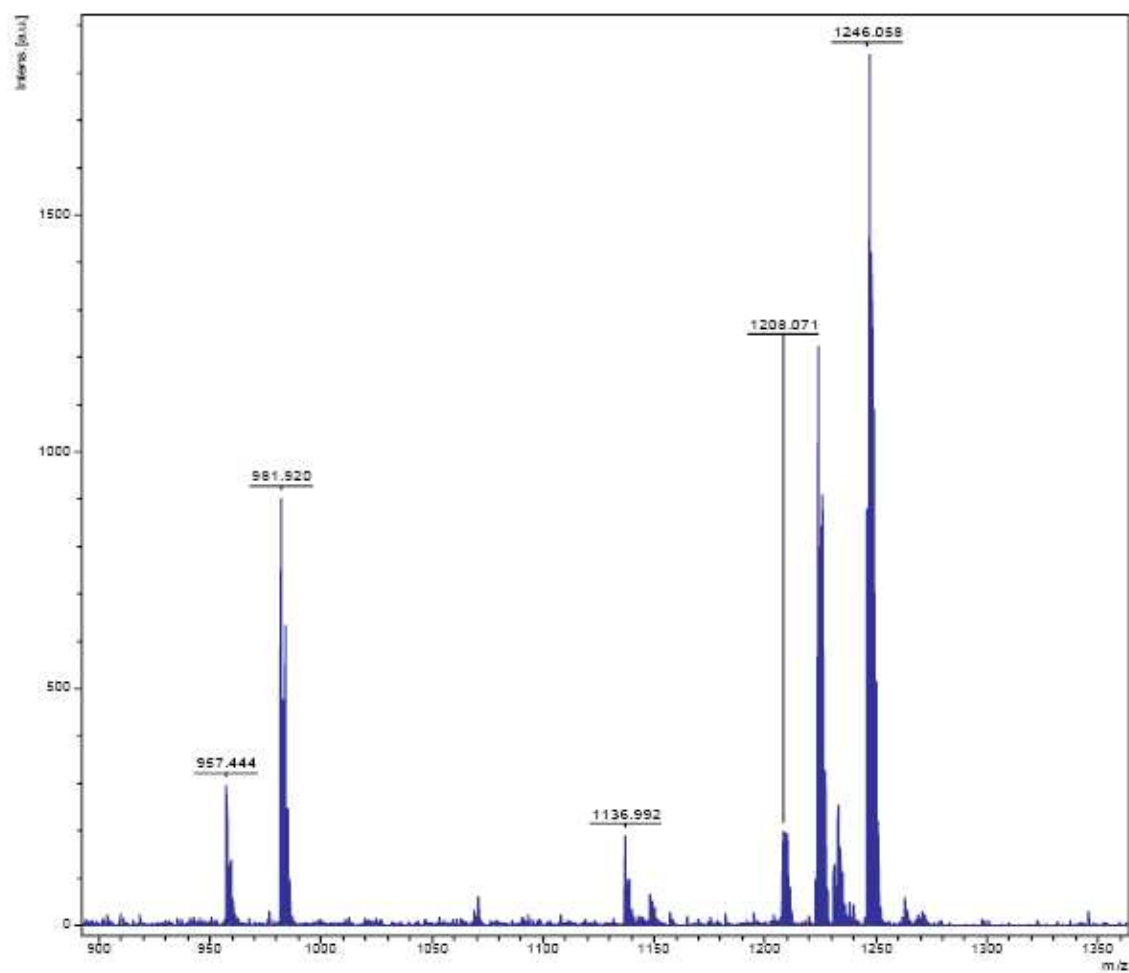


Figure S6. Mass spectrum (MALDI) of CT02-AT.

D:\DATA\MALDI\Dec 09\M121009\15149 CT02 VER TEMPO\0_F6\1

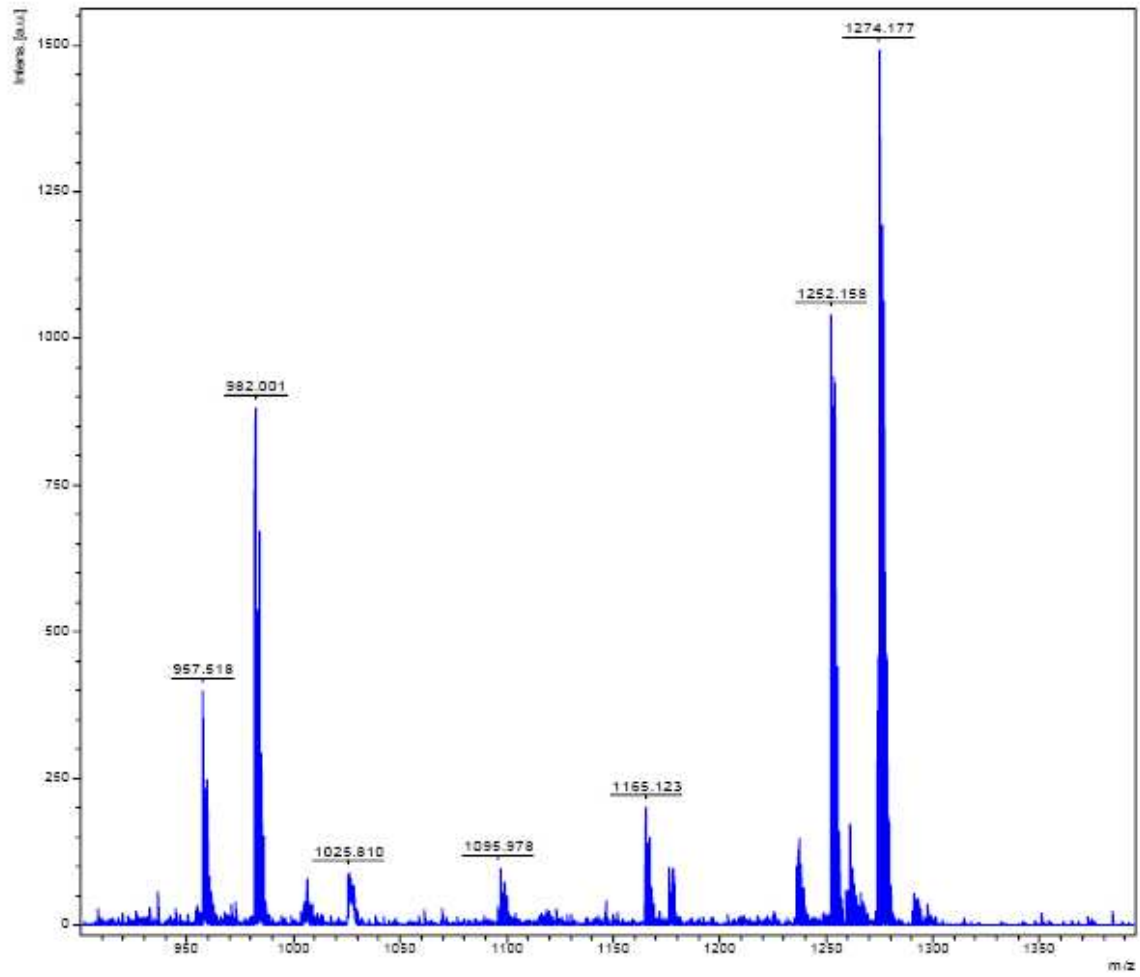


Figure S7. Mass spectrum (MALDI) of CT02-VT.

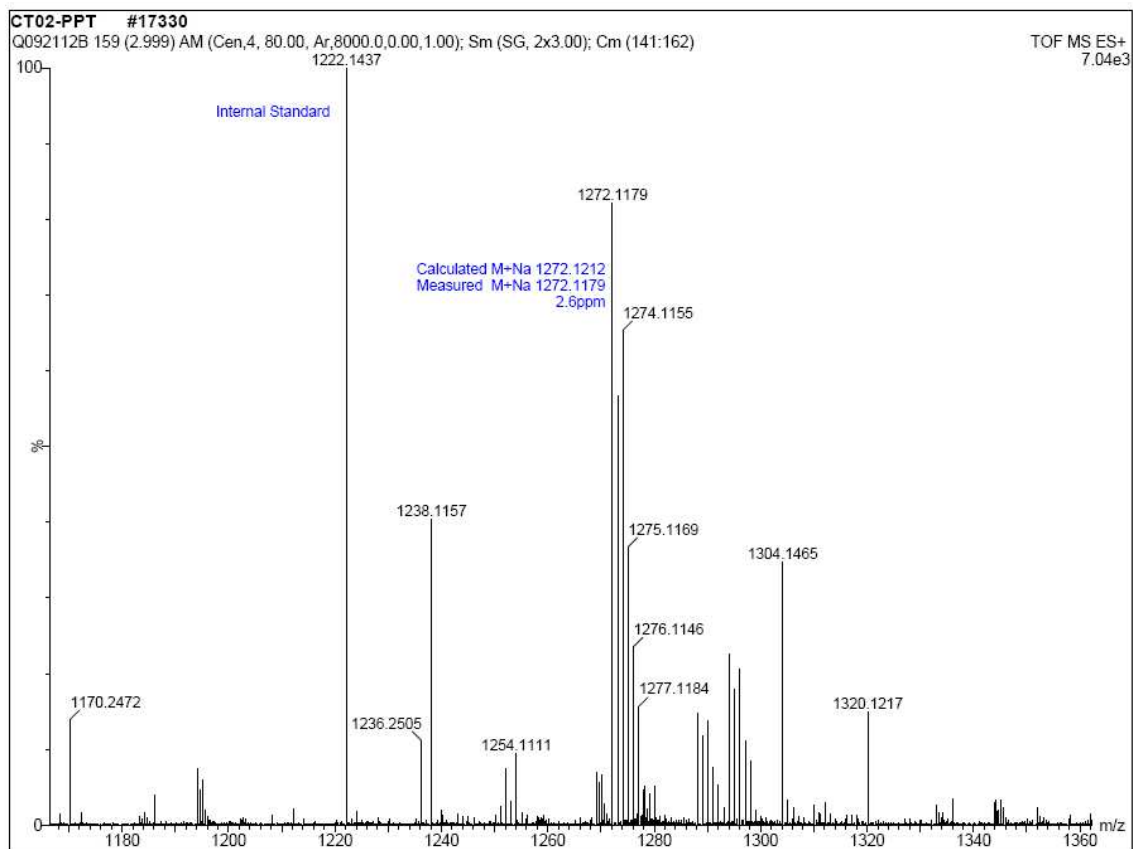


Figure S8. Mass spectrum (ESI) of CT02-PPT.

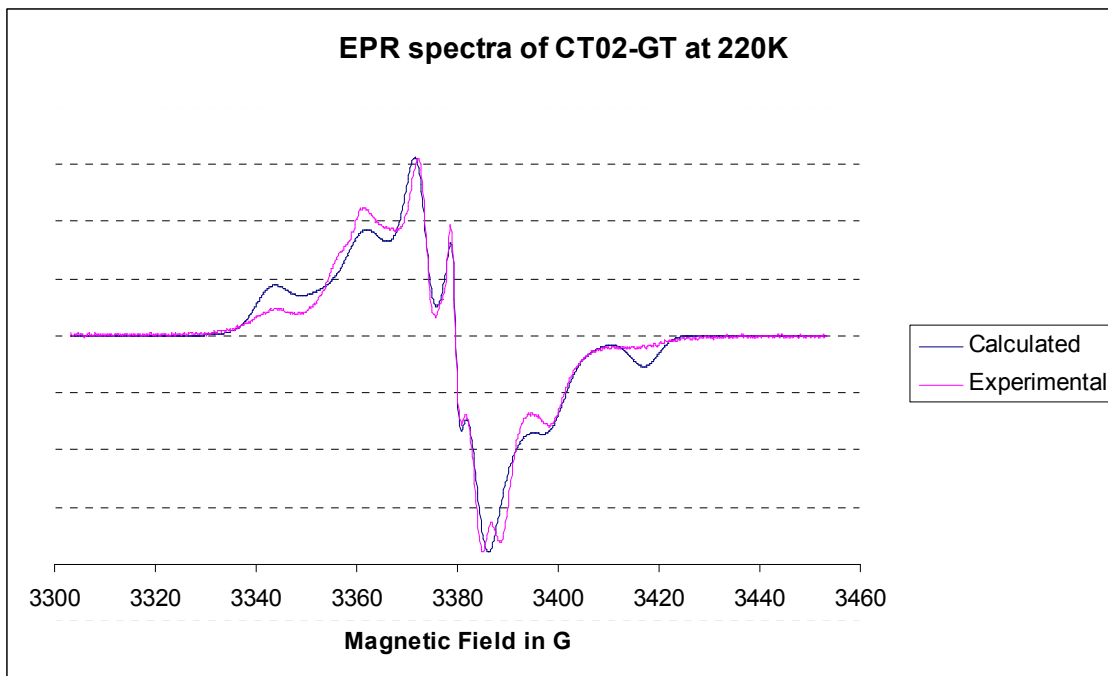


Figure S9. Experimental and simulated EPR spectra of CT02-GT at 220 K in ethylene glycol/H₂O(1:1, v/v) glass-forming solution.

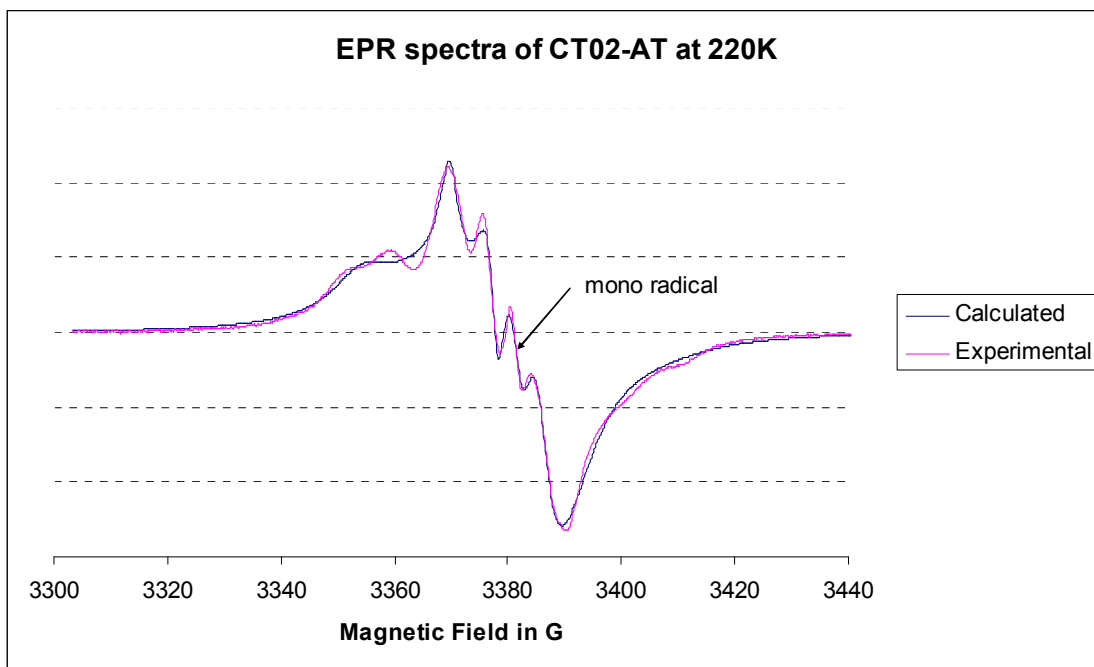


Figure S10. Experimental and simulated EPR spectra of CT02-AT at 220 K in ethylene glycol/H₂O(1:1, v/v) glass-forming solution.

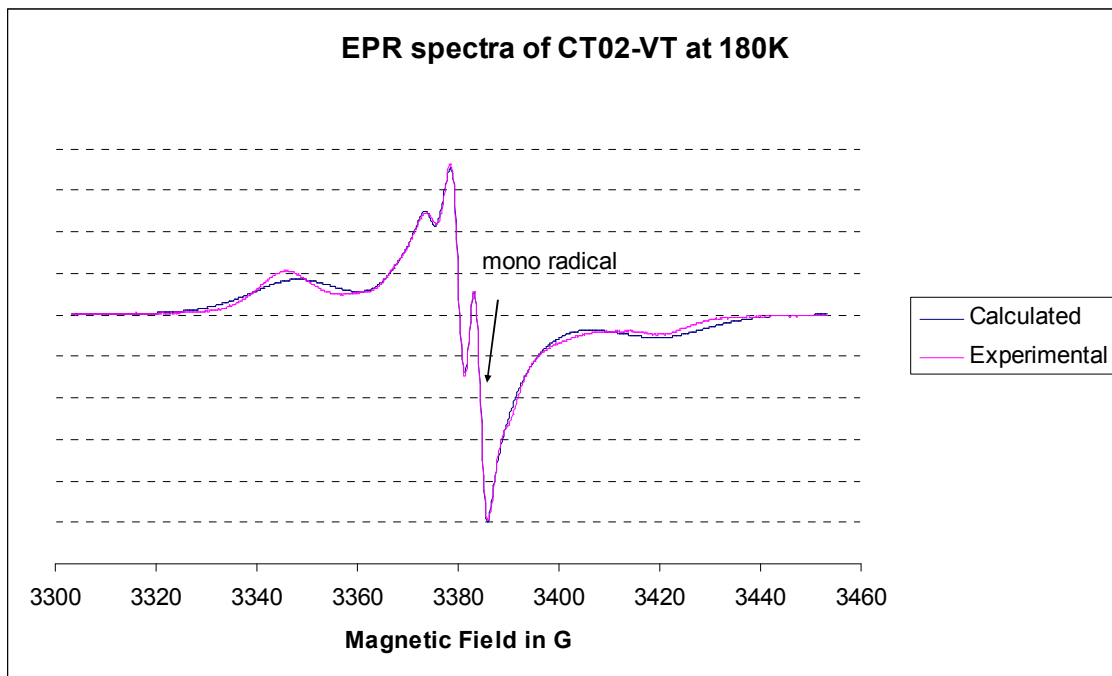


Figure S11. Experimental and simulated EPR spectra of CT02-VT at 180 K in ethylene glycol/H₂O(1:1, v/v) glass-forming solution.

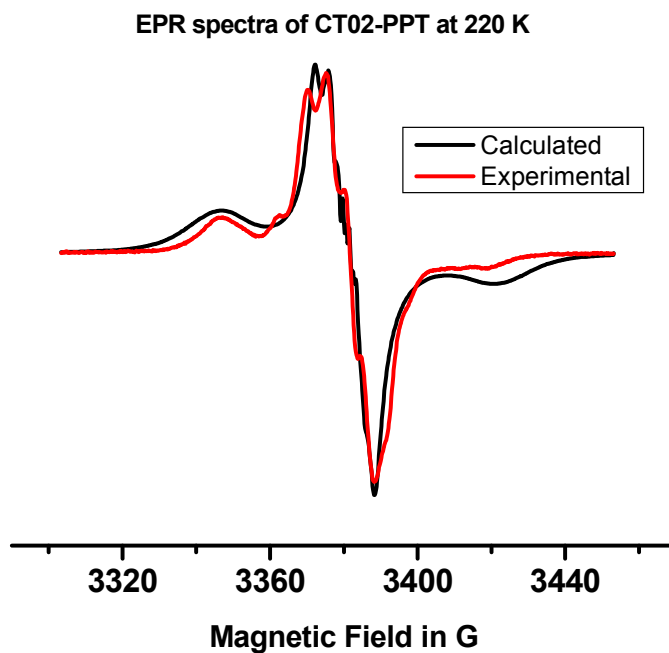


Figure S12. Experimental and simulated EPR spectra of CT02-PPT at 220 K in ethylene glycol/H₂O(1:1, v/v) glass-forming solution.

The Cartesian coordinates for two conformers of CT02-PPT were generated using the GaussView 3.0 Program.

Conformer 1

C	-3.06912100	-2.55218100	0.20510500
C	-1.77623400	-1.77944300	0.06687400
O	-3.04223400	-3.67612100	0.63244900
C	-1.45146900	-0.76449300	0.95237300
C	-0.19908100	-0.16697100	0.93064200
C	0.76833900	-0.56707200	0.00902200
C	0.42633700	-1.57159900	-0.90063700
C	-0.82389900	-2.17082400	-0.86033600
C	2.10792000	0.05731100	0.00014300
C	2.20678100	1.53288200	0.03782100
C	3.31242900	-0.80181300	-0.03498200
C	1.46729200	2.30430200	-0.85401500
C	1.51112300	3.69331100	-0.81544200
C	2.29277700	4.35134300	0.13457900
C	3.04611100	3.57973000	1.03081100
C	3.00033700	2.19160600	0.97754400
C	3.45091900	-1.85741000	0.86041200
C	4.55354700	-2.70291000	0.81294800
C	5.54974500	-2.51721600	-0.14664500
C	5.42051200	-1.44844400	-1.04414500
C	4.31764600	-0.60630500	-0.98134900
S	2.23462500	-2.24400900	2.08076400
C	3.32862200	-3.27611300	3.11498600
S	4.57098100	-4.01728800	2.00207000
S	6.53714800	-1.13012100	-2.39285300
C	5.96597200	0.56259900	-2.75002400
S	4.22496100	0.66046400	-2.21049300
S	1.49837300	-2.13689300	-2.18751900
C	0.55729200	-3.64506100	-2.63270900
S	-1.17543200	-3.36219200	-2.11984600
S	-2.58537900	-0.18912000	2.18508100
C	-1.35258200	0.68718200	3.21680100
S	0.04342400	1.12390300	2.11522600
C	0.30436700	3.08786200	-3.11387600
S	0.50011500	4.52776500	-2.00839800
S	4.01201200	4.25065500	2.36616000
C	4.96551600	2.73917200	2.72189500
S	3.93337400	1.32554100	2.20342400
S	0.38746500	1.59942200	-2.06085400
C	6.29078400	2.74788300	1.95630000

C	5.21782300	2.65013200	4.22662600
C	4.00675800	-2.42804700	4.19263800
C	2.50295000	-4.39267100	3.75272700
C	6.81923800	1.58712800	-1.99850100
C	6.03948200	0.80761300	-4.25686400
C	0.60873300	-3.83324700	-4.14777600
C	1.13261500	-4.86746000	-1.91394300
C	-1.97643900	1.97286300	3.75628200
C	-0.88290800	-0.20923500	4.36376600
C	1.40919400	3.06349600	-4.17104800
C	-1.07041300	3.15299700	-3.77711200
C	6.68415500	-3.49444800	-0.16744000
C	2.25347800	5.84864700	0.14596800
O	3.10280800	6.41840800	0.94726000
O	7.64821200	-3.20542500	-0.98925400
O	6.72436400	-4.49363400	0.48605000
O	1.49293700	6.50589800	-0.49913700
N	-4.20351200	-1.91277100	-0.16642400
C	-5.46780000	-2.56772600	0.09232800
C	-6.32591400	-2.52142300	-1.15918200
N	-6.45355100	-1.17159300	-1.66721400
C	-5.15447500	-0.66827000	-2.04494400
C	-4.26462300	-0.60394000	-0.81586600
C	-7.53289400	-0.34846500	-1.78784900
C	-8.93360600	-0.66479400	-1.18715300
C	-9.10910300	-1.39705800	0.18350400
C	-9.42969900	-0.47358600	1.39443000
N	-8.88238600	0.88563100	1.13830200
C	-9.44697000	1.63195300	-0.02417100
C	-9.76908100	0.63392100	-1.16437700
O	-7.45092400	0.62196800	-2.49533400
O	-7.59222200	0.79502900	1.06587600
C	-8.78306200	-1.00022900	2.67879000
C	-10.94253500	-0.45938400	1.67126200
C	-8.47065800	2.74282200	-0.42895400
C	-10.73486100	2.37371800	0.38817600
H	6.12049100	2.81432800	0.89228300
H	6.89482200	3.59548300	2.26052300
H	6.84661600	1.83969800	2.16038800
H	5.76868700	1.74608300	4.45827600
H	5.81423700	3.49356600	4.55499900
H	4.29154100	2.64321800	4.78008100
H	4.60326300	-1.64389700	3.75071100
H	3.26227800	-1.97177900	4.83513900
H	4.65400000	-3.04945400	4.80185700
H	1.74612600	-3.97265600	4.40467600

H	2.01649400	-4.99914100	3.00417800
H	3.14196000	-5.02818900	4.35486900
H	6.77530500	1.41777600	-0.93317300
H	7.85419300	1.51725800	-2.31423200
H	6.46504300	2.59116000	-2.20279300
H	7.06621600	0.73442800	-4.59651900
H	5.44151000	0.09241700	-4.80031500
H	5.68546200	1.80488200	-4.48896100
H	0.20484100	-2.97639900	-4.66434000
H	1.63274400	-3.98305600	-4.46925700
H	0.04075800	-4.71163100	-4.43144700
H	2.16383600	-5.02221400	-2.21085800
H	1.09989000	-4.73873100	-0.84260200
H	0.56389100	-5.75381900	-2.17118000
H	-2.31333200	2.61229400	2.95536300
H	-2.82111000	1.73701500	4.39289100
H	-1.25168600	2.51414500	4.35317800
H	-1.71932900	-0.46247500	5.00570100
H	-0.45059800	-1.12379500	3.98777800
H	-0.13697500	0.30717400	4.95732100
H	2.38591800	3.03656900	-3.71169500
H	1.30364900	2.19023800	-4.80448900
H	1.34709900	3.95071200	-4.79153300
H	-1.14459100	4.04476900	-4.38836600
H	-1.21398400	2.29519700	-4.42348000
H	-1.86102700	3.17010200	-3.04242100
H	2.98132000	7.34806000	0.89108800
H	8.29242200	-3.88710900	-0.93732700
H	-5.25006400	-3.58071800	0.37961300
H	-5.96049100	-2.06492800	0.91302300
H	-5.81939800	-3.10190000	-1.92333500
H	-7.28796800	-2.97847400	-1.02124200
H	-5.27348600	0.29422000	-2.50553400
H	-4.71627400	-1.35098000	-2.76371800
H	-4.65691800	0.13003300	-0.12666000
H	-3.26679600	-0.31491100	-1.10330600
H	-9.35597700	-1.28906700	-1.96600000
H	-8.26144100	-2.00644700	0.42686100
H	-9.94105700	-2.08603700	0.08974800
H	-9.70369600	1.13440500	-2.11405500
H	-10.79969700	0.32031900	-1.05792100
H	-9.05201600	-0.36693300	3.51461100
H	-9.13805700	-2.00350600	2.88042400
H	-7.70781200	-1.02795600	2.61202900
H	-11.20980600	-1.42527400	2.07746500
H	-11.55308300	-0.30920900	0.79677200

H	-8.88423200	3.26409800	-1.27998900
H	-8.36711500	3.44366500	0.39118600
H	-7.49540900	2.38924000	-0.69754100
H	-11.04184500	3.01723800	-0.42611600
H	-11.56904200	1.73158800	0.61481300
H	-10.54294700	2.99305000	1.25453700
H	-11.19963400	0.29253000	2.40545300

Conformer 2

C	-3.23529500	-1.49393600	0.84812000
C	-1.83967100	-0.99599600	0.54485000
O	-3.39443400	-2.61041200	1.26554400
C	-1.21874300	-0.06789500	1.36571800
C	0.11748000	0.26311800	1.19315600
C	0.87309000	-0.32329100	0.17793800
C	0.23366400	-1.23359300	-0.66850600
C	-1.09858700	-1.56829000	-0.47657600
C	2.30077100	0.01448200	0.00878100
C	2.70028800	1.43773800	0.01128000
C	3.29248300	-1.07120000	-0.14769400
C	2.03485700	2.35052400	-0.80169400
C	2.36380900	3.70139600	-0.79019500
C	3.36632000	4.17885700	0.05454300
C	4.04593000	3.26291600	0.87046400
C	3.71329400	1.91390100	0.84438800
C	3.31204600	-2.14073400	0.74173300
C	4.20604000	-3.19325500	0.58351300
C	5.10429500	-3.20666400	-0.48464800
C	5.09627900	-2.12627400	-1.37722800
C	4.20295400	-1.07720400	-1.20363100
S	2.18758900	-2.28130300	2.09552200
C	3.15727800	-3.52375100	3.01606000
S	4.08886000	-4.49375300	1.78198200
S	6.09492400	-2.03166200	-2.84687600
C	5.84493700	-0.25487600	-3.16236200
S	4.23215600	0.19149000	-2.43343200
S	1.01576700	-1.99728900	-2.05723600
C	-0.25342800	-3.28327800	-2.36298300
S	-1.82389800	-2.65348800	-1.66990500
S	-2.06453600	0.72607700	2.70442200
C	-0.56859600	1.31849600	3.57817300
S	0.74861700	1.47503100	2.31647400
C	0.80394200	3.37254900	-2.92567900

S	1.41217900	4.73379100	-1.87181000
S	5.27526700	3.71246000	2.07544200
C	5.93599400	2.03539500	2.34308500
S	4.58459400	0.86658300	1.96984900
S	0.70244700	1.89040900	-1.86499100
C	7.13756100	1.77975800	1.43016800
C	6.33775000	1.88533700	3.80997800
C	4.11123800	-2.84150900	3.99843700
C	2.19833000	-4.45368900	3.75838800
C	6.96807700	0.56689900	-2.52564300
C	5.79719900	-0.01695200	-4.67138400
C	-0.41109300	-3.47610800	-3.87003500
C	0.13983600	-4.59759500	-1.68495700
C	-0.84953600	2.69779300	4.17123000
C	-0.16370500	0.33004700	4.67286400
C	1.75309300	3.13151700	-4.10011100
C	-0.59527700	3.72098500	-3.43074000
C	6.00476600	-4.39649100	-0.61889000
C	3.63175000	5.65363000	0.04855700
O	4.66417800	6.03233200	0.74166700
O	6.90739700	-4.30433700	-1.54985500
O	5.91340300	-5.38929300	0.03959500
O	2.95097500	6.45778800	-0.51481800
N	-4.24640300	-0.61982500	0.63261500
C	-5.58805400	-0.97659800	1.01578200
C	-6.51108800	-0.94552100	-0.19179600
N	-6.43563500	0.34822200	-0.85123900
C	-5.08399900	0.68378900	-1.24273500
C	-4.15388800	0.66318900	-0.04189100
C	-7.42143200	1.24511200	-1.14326100
C	-8.88630500	0.96521500	-0.79873400
C	-9.48055700	-0.24733000	-1.57663500
C	-10.84520700	-0.74556600	-1.06129200
N	-10.83187800	-0.77713000	0.42793400
C	-10.51826300	0.47728700	1.16977500
C	-9.13001800	0.98151100	0.73791800
O	-7.16154500	2.29107600	-1.68137500
O	-10.02253400	-1.71512300	0.82426900
C	-11.11678100	-2.17499800	-1.54160900
C	-11.98322200	0.12649500	-1.62220100
C	-10.53202100	0.13555800	2.66333900
C	-11.57578400	1.57513500	0.96055700
H	6.86181400	1.88803300	0.39220300
H	7.93218100	2.48419400	1.64940800
H	7.51635700	0.77556500	1.58321100
H	6.71602900	0.88626100	3.99116200

H	7.12729200	2.58673800	4.05332100
H	5.50009600	2.06341300	4.46620300
H	4.80135100	-2.19220100	3.48095900
H	3.55281000	-2.24842200	4.71363900
H	4.68248900	-3.58755900	4.53978900
H	1.62123000	-3.89370300	4.48476200
H	1.51791600	-4.94165200	3.07792300
H	2.75830100	-5.21119400	4.29413700
H	7.01011000	0.40042300	-1.45976000
H	7.92473800	0.28971900	-2.95419000
H	6.80523700	1.62380200	-2.70371200
H	6.74280800	-0.29531000	-5.12205100
H	5.00898800	-0.59033200	-5.13414300
H	5.63001600	1.03372100	-4.87669400
H	-0.68821600	-2.55440100	-4.35736600
H	0.51890500	-3.83089300	-4.29811700
H	-1.17310100	-4.22041300	-4.07002800
H	1.07877100	-4.95809400	-2.08983500
H	0.25373300	-4.46583200	-0.61965600
H	-0.62165100	-5.34933000	-1.85823600
H	-1.13816300	3.40278100	3.40733000
H	-1.64467600	2.63155600	4.90472500
H	0.03459900	3.07127100	4.67386600
H	-0.95422600	0.24552800	5.41038600
H	0.02518900	-0.64860100	4.25953500
H	0.73604000	0.67492700	5.16933600
H	2.74947500	2.90354300	-3.75314500
H	1.40124500	2.30242800	-4.70296300
H	1.80180300	4.01726900	-4.72382000
H	-0.55563100	4.61337000	-4.04387500
H	-0.98205200	2.91542700	-4.04363100
H	-1.27719200	3.89323000	-2.61201700
H	4.72654300	6.96791700	0.68676900
H	7.39858400	-5.10478500	-1.56178900
H	-5.55984700	-1.95212100	1.46544600
H	-5.93163200	-0.25665300	1.75083600
H	-6.19407800	-1.71260400	-0.89032100
H	-7.51365400	-1.16211700	0.11570100
H	-5.10197700	1.65307500	-1.70365900
H	-4.73914100	-0.04660700	-1.96802300
H	-4.43423900	1.45133500	0.64492200
H	-3.13918600	0.82818400	-0.36215800
H	-9.33929500	1.85230600	-1.20555800
H	-8.79143700	-1.07715500	-1.60646900
H	-9.60458700	0.05504900	-2.60957400
H	-8.37513100	0.41425700	1.26068500

H	-9.01515400	2.00227700	1.08208700
H	-12.06908500	-2.52278100	-1.16097200
H	-11.15369100	-2.18550300	-2.62322300
H	-10.35104200	-2.86298500	-1.22268500
H	-12.15251400	-0.16611200	-2.64857500
H	-11.76439500	1.18151000	-1.63437000
H	-11.50633900	-0.23828400	2.95272100
H	-9.79369300	-0.60821700	2.91561200
H	-10.32312300	1.02985900	3.23577700
H	-11.47477400	2.29098900	1.76361000
H	-11.46283500	2.12521500	0.04089400
H	-12.57872100	1.17176900	0.99986900
H	-12.90455300	-0.02794100	-1.07674500