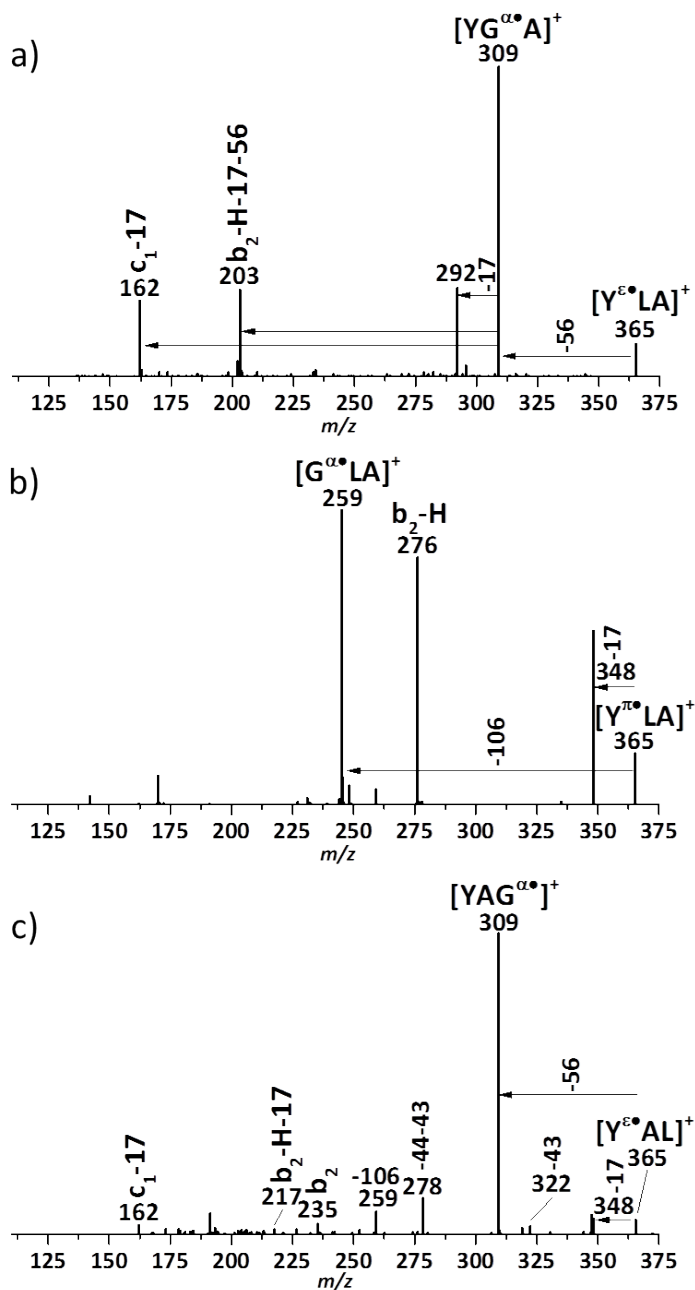


## SUPPLEMENTARY INFORMATION

Figure S1. CID spectra of a)  $[\text{Y}^{\varepsilon}\text{LA}]^+$ , b)  $[\text{Y}^{\pi}\text{LA}]^+$ , c)  $[\text{Y}^{\varepsilon}\text{AL}]^+$ , d)  $[\text{Y}^{\pi}\text{AL}]^+$  and e)  $[\text{Y}^{\varepsilon}\text{GI}]^+$ .



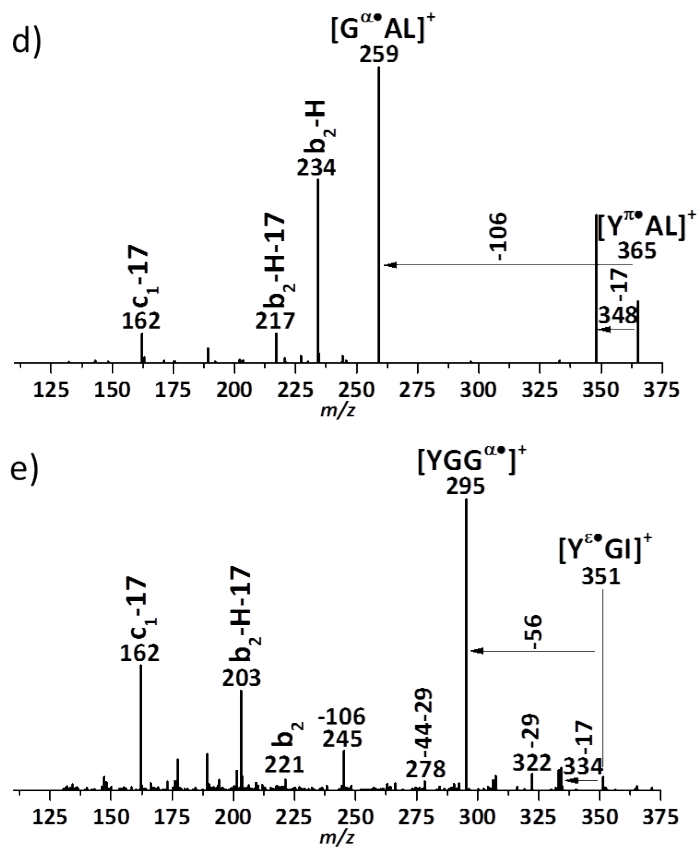


Figure S2. CID spectrum of  $[YGG^{\alpha}-18]^+$  from CID spectrum of  $[YGG^{\alpha}]^+$

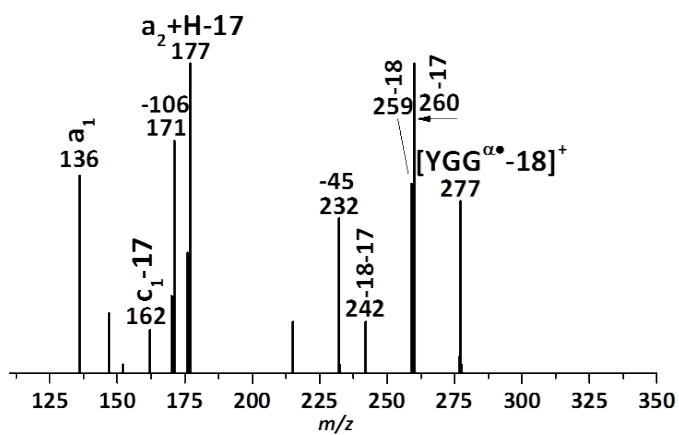


Figure S3. CID spectra of a)  $[Y^{\epsilon}\text{AG}]^+$ , b)  $[Y\text{G}^{\alpha}\text{A}]^+$  and c)  $[Y\text{AG}^{\alpha}]^+$ .

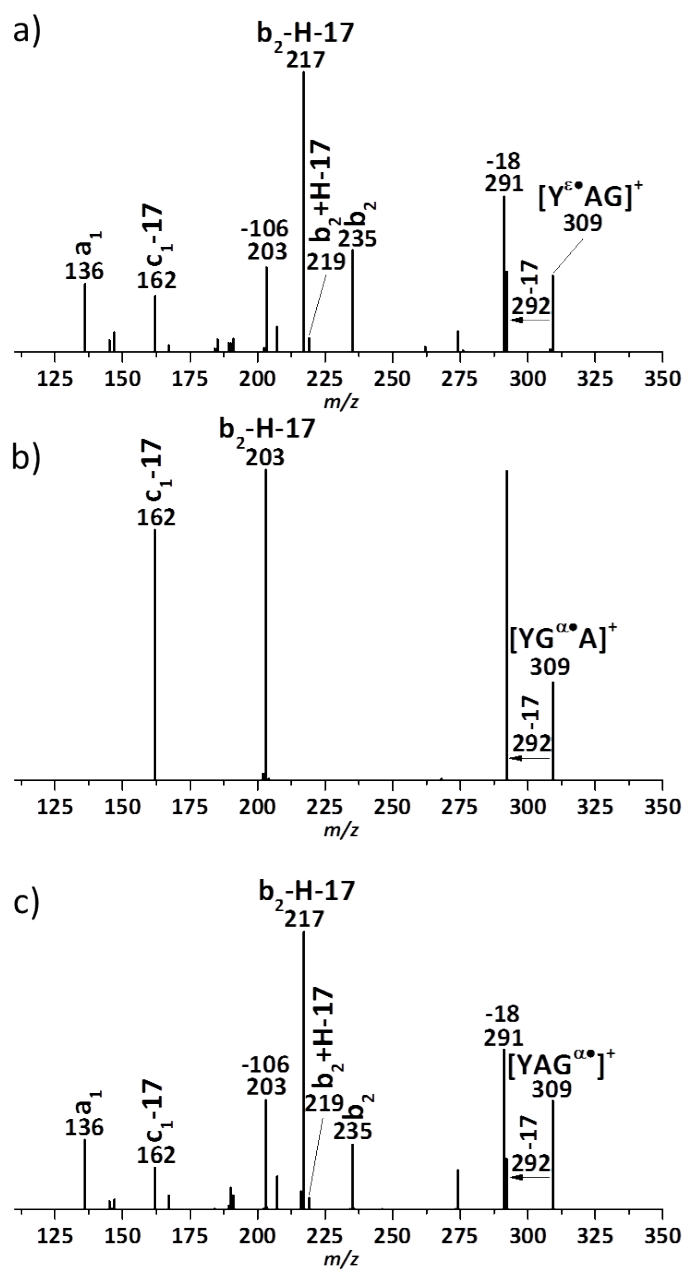


Figure S4. CID spectra of  $[\text{YG}^{\alpha}\text{G-NH}_3]^+$ .

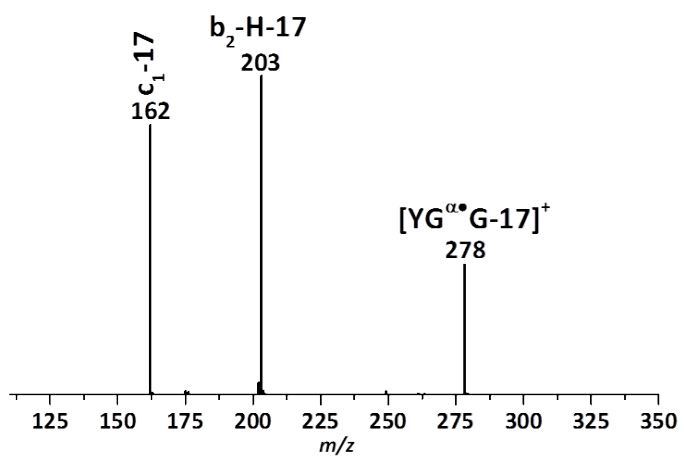


Table S1. Coordinates for Figure 4a

[Y<sup>π</sup>GG]<sup>+</sup>

N	0.83562100	3.25270600	0.01630100
C	1.59142100	2.06881000	-0.26447500
C	0.73829100	0.77694100	-0.11250200
C	2.89380000	1.88016500	0.58636800
N	-0.57874600	0.93698200	-0.11103700
O	1.31292100	-0.32443600	-0.04360500
C	3.60578900	0.59176100	0.31513000
C	4.21583500	0.35321500	-0.95269900
C	4.95851200	-0.77786600	-1.18460400
C	5.13168500	-1.72366200	-0.13865100
C	4.55681100	-1.50368000	1.13726400
C	3.81092600	-0.36801100	1.35080000
O	5.86148500	-2.80105900	-0.42963800
C	-1.53487000	-0.15399500	-0.05407100
C	-2.93736000	0.47418700	-0.05530000
N	-3.96952400	-0.39397400	-0.01864800
O	-3.07476900	1.69623700	-0.08840300
C	-5.34916000	0.07750700	-0.02062300
C	-6.36950700	-1.04375100	-0.00009500
O	-7.56028200	-0.85439200	0.00223400
O	-5.80462100	-2.27889200	0.01574500
H	0.79146100	3.52599800	0.99210800
H	1.02987000	4.04994100	-0.57615600
H	3.54894600	2.72494700	0.34182300
H	2.63793800	1.95865000	1.64801800
H	-0.96634900	1.88163500	-0.17164400
H	4.10107800	1.08460700	-1.74699400
H	5.43019500	-0.97054000	-2.14188100
H	4.70440300	-2.22876700	1.93276400
H	3.36097500	-0.19637000	2.32316200
H	-6.52336100	-2.93512900	0.02724800
H	-1.41022500	-0.82143200	-0.91497600
H	-1.38015200	-0.75216900	0.85162700
H	-3.81228100	-1.39314000	-0.00031100
H	-5.54109100	0.71730800	0.84764500
H	-5.54617300	0.69081400	-0.90664600

H	5.94780800	-3.40595100	0.32451200
H	1.86457200	2.09020800	-1.32653000
[Y <sup>*</sup> GG] <sup>+</sup>			
N	0.46807200	0.57942900	0.74997500
C	0.42579300	-0.71881100	-0.01874200
C	-0.89555400	-1.35654000	0.44234600
O	-1.22805200	-1.21199000	1.62290300
H	1.39892000	1.00879000	0.68648500
H	0.24541700	0.35256500	1.73068500
H	0.40572700	-0.45248400	-1.07868500
C	1.67599300	-1.56736000	0.31010300
C	2.96839500	-0.81190600	0.07461900
H	1.62694000	-2.46797700	-0.31147900
H	1.60982800	-1.89959100	1.35229000
C	5.36547500	0.66828500	-0.34724300
C	3.68094400	-0.24256900	1.14558300
C	3.48007400	-0.63722200	-1.23202700
C	4.63513500	0.08828100	-1.37321900
C	4.85682200	0.48583700	0.95004500
H	3.33539900	-0.40227800	2.16470400
H	2.98652200	-1.08119700	-2.09414800
H	5.40567600	0.90389900	1.78885600
O	6.50743400	1.37703600	-0.50716700
H	6.77080100	1.39328800	-1.43877100
N	-1.63099300	-2.00103100	-0.48305000
C	-3.05002500	-2.30198900	-0.23728400
C	-3.82422000	-1.00106600	-0.51160600
O	-4.25093600	-0.73811800	-1.62706400
H	-1.34361900	-1.95476600	-1.45295500
H	-3.37848000	-3.06615600	-0.94046300
H	-3.15924900	-2.66673500	0.78530000
N	-3.88580900	-0.13317100	0.54617900
C	-4.28479300	1.23758700	0.34942700
C	-3.12351800	2.16637700	0.00516800
O	-1.93662200	1.86100800	-0.00446200
O	-3.55976900	3.39132800	-0.27675200
H	-3.40928400	-0.38623800	1.40291700

H	-5.00956400	1.28800900	-0.46803500
H	-4.77633800	1.63186800	1.24506300
H	-0.27887800	1.22240600	0.42363800
H	-2.80826600	3.97245700	-0.48981200

[YGG<sup>α</sup>]<sup>+</sup>

N	2.32488600	1.95419000	-0.90127500
C	1.44786800	0.75796100	-0.61639400
C	0.06540300	1.38466800	-0.32137300
O	0.02313300	2.59318700	-0.05102200
H	1.81324600	2.75245500	-0.45266400
H	2.41388700	2.15429100	-1.90004300
H	1.43492300	0.12758800	-1.50826500
C	2.01740600	-0.02430600	0.59809400
C	3.48948700	-0.34293000	0.44623000
H	1.42101400	-0.93698000	0.69961400
H	1.84792700	0.56523100	1.50639300
C	6.23810800	-0.88419600	0.12174500
C	3.93055900	-1.34631300	-0.43751100
C	4.45640700	0.37667200	1.16566200
C	5.82115700	0.11493700	1.00888400
C	5.28280400	-1.61769000	-0.60198700
H	3.20699100	-1.94206800	-0.98961900
H	4.14858200	1.12572100	1.89285500
H	6.55053900	0.67380600	1.58922900
H	5.62181200	-2.40105400	-1.27133000
O	7.53932400	-1.20344600	-0.08678800
H	8.12743600	-0.68576800	0.48063300
N	-0.98541600	0.56610700	-0.34104700
C	-2.33984500	0.99658800	-0.03139700
C	-3.23485200	-0.23499200	-0.19725800
O	-2.76477300	-1.31952300	-0.53066800
H	-0.91741100	-0.42030200	-0.59251200
H	-2.39677100	1.38694600	0.99177300
H	-2.65230100	1.80110800	-0.70791100
N	-4.56501900	-0.03267300	0.04919500
C	-5.53301600	-0.99800500	-0.04197000
C	-6.87730100	-0.55570300	0.26378600

O	-7.13495200	0.60217100	0.58278700
O	-7.79557900	-1.53649800	0.16120200
H	-4.91239400	0.88648100	0.32367500
H	-5.25331600	-2.00142600	-0.32706500
H	3.26665100	1.81218000	-0.50700500
H	-8.66431200	-1.15883800	0.38097400

[YG<sup>o</sup>G]<sup>+</sup>

N	2.33206900	1.93713900	-0.93584300
C	1.45734300	0.74838100	-0.60995600
C	0.07999200	1.37670500	-0.33033000
O	0.02142400	2.58205500	-0.05591400
H	1.85525700	2.74663400	-0.47798900
H	2.38465800	2.12879800	-1.93920100
H	1.44833700	0.08950300	-1.48158500
C	2.04190300	0.00645600	0.62478900
C	3.51271800	-0.31423300	0.46551200
H	1.44873300	-0.90375000	0.76218700
H	1.87997400	0.62560400	1.51447500
C	6.25838900	-0.86121100	0.12672300
C	3.94519300	-1.34904400	-0.38581200
C	4.48682100	0.43433100	1.14506100
C	5.85009200	0.16977100	0.98095600
C	5.29599600	-1.62338700	-0.55698300
H	3.21626900	-1.96700500	-0.90551700
H	4.18613600	1.20919700	1.84776900
H	6.58527500	0.75130300	1.53090200
H	5.62864300	-2.43068400	-1.20057800
O	7.55751400	-1.18543600	-0.08599200
H	8.15159600	-0.64587100	0.45420200
N	-0.98469700	0.54327000	-0.36159700
C	-2.28269900	0.87886200	-0.07797600
C	-3.20759700	-0.25116700	-0.21002800
O	-2.76031100	-1.36226500	-0.54817400
H	-0.89763000	-0.44684500	-0.61680700
H	-2.51509500	1.89575800	0.20674800
N	-4.51312400	-0.01351200	0.04776200
C	-5.51620000	-1.05420600	-0.05353400



C	-6.86565900	-0.45247600	0.28640700
O	-7.03211000	0.71136400	0.58767300
O	-7.84262600	-1.36618400	0.21173000
H	-4.85016500	0.90495400	0.31928700
H	-5.54813100	-1.48089000	-1.06305900
H	-5.30204800	-1.88390100	0.63062700
H	3.28627800	1.78666800	-0.57429400
H	-8.68670500	-0.93671600	0.43702700

TS<sub>[Y<sub>g</sub>•GG]<sup>+</sup>→[Y<sub>π</sub>•GG]<sup>+</sup></sub>

N	-3.48203000	-3.24193100	-0.17528600
C	-2.91682700	-1.95800400	-0.55921400
C	-1.73770200	-1.67568800	0.38292800
C	-3.90019300	-0.73463200	-0.53603500
N	-0.48523600	-1.65555300	-0.20731600
O	-1.89379100	-1.42084300	1.56761400
C	-3.17160700	0.59102300	-0.44066600
C	-2.07678300	0.86037500	-1.27005200
C	-1.15484100	1.81591700	-0.85318300
C	-1.46520600	2.79806500	0.10820200
C	-2.62490000	2.59790800	0.87799300
C	-3.43473600	1.49877600	0.61251100
O	-0.61599800	3.82993200	0.26824300
C	0.68484500	-1.39478900	0.59499300
C	1.62123400	-0.36160600	-0.00966600
N	2.91938700	-0.57681600	0.09390000
O	1.25890900	0.72179900	-0.59149800
C	3.93912200	0.37555200	-0.35977600
C	5.35484900	-0.09329000	-0.06081900
O	6.32627300	0.55860900	-0.33753800
O	5.38244600	-1.30884300	0.53740500
H	-3.85492600	-3.21649900	0.77045200
H	-4.21609600	-3.54209000	-0.80974700
H	-4.52837200	-0.78928000	-1.43358200
H	-4.55754600	-0.84479300	0.33113500
H	-0.37228300	-2.10889000	-1.10462000
H	-1.84737500	0.21003600	-2.10961100
H	0.21674300	1.07847900	-0.65715500

H	-2.89302500	3.30445900	1.66027800
H	-4.30627700	1.33179200	1.23888500
H	6.31017400	-1.55629200	0.70197700
H	0.31998300	-1.01154800	1.55853300
H	1.25591700	-2.30659400	0.80980200
H	3.25337700	-1.43518900	0.52088600
H	3.85348400	0.53494700	-1.43925900
H	3.78891600	1.34638300	0.12195700
H	-0.92156100	4.43192600	0.96377000
H	-2.53222300	-2.06963800	-1.57990000

TS<sub>[Y<sub>g</sub>•GG]<sup>+</sup>→[YO•GG]<sup>+</sup></sub>

N	2.46320600	2.05149500	-0.77552300
C	1.57503200	0.84924100	-0.54942200
C	0.18598800	1.48534800	-0.27628600
C	2.08266700	0.01804200	0.65883200
N	-0.86512500	0.67530000	-0.32063200
O	0.15564200	2.69539900	-0.00587000
C	3.52816000	-0.39987200	0.50895600
C	4.54607700	0.40084000	1.07769600
C	5.88166400	0.13675400	0.77751400
C	6.14642100	-1.04612400	0.00404200
C	5.15789000	-1.92625400	-0.51801900
C	3.85204300	-1.55824200	-0.26928800
O	7.44242600	-1.13016800	-0.06939600
C	-2.22977900	1.09462900	-0.03653000
C	-3.09881800	-0.16550700	-0.19313600
N	-4.41230100	-0.00707100	0.03033300
O	-2.57414400	-1.23779400	-0.50851600
C	-5.35875100	-1.10361600	-0.08203600
C	-6.74305700	-0.56675200	0.22819800
O	-6.96920900	0.59033900	0.51642000
O	-7.67166700	-1.52724000	0.14331200
H	2.60276100	2.25871500	-1.76729200
H	1.90455900	2.83931700	-0.35155400
H	1.57755800	0.24641400	-1.46046000
H	1.95211000	0.60902400	1.57271600
H	1.42782000	-0.85509300	0.74417300

H	-0.80580600	-0.31576100	-0.56746300
H	4.27063100	1.22366100	1.73910400
H	3.38629700	1.93936900	-0.33411800
H	5.41709400	-2.83262000	-1.05474300
H	3.04189900	-2.17915900	-0.64394200
H	-8.54077400	-1.13984200	0.34954700
H	-2.30543200	1.50092300	0.97799700
H	-2.54662300	1.87746300	-0.73463000
H	-4.81072600	0.89174200	0.28727200
H	-5.34970200	-1.53613200	-1.08879300
H	-5.11509200	-1.91359300	0.61464900
H	7.37536700	-0.08771800	0.58756700

TS<sub>[Y $\beta$ •GG]<sup>+</sup>→[YG $\alpha$ •G]<sup>+</sup></sub>

N	-2.73074600	-3.34687400	-0.19718500
C	-2.31263800	-1.93584400	-0.60122000
C	-1.43709200	-1.49762000	0.61496500
C	-3.62032200	-1.09054000	-0.79223100
N	-0.29400200	-0.77038800	0.53227400
O	-1.83736200	-1.92458900	1.70647000
C	-3.25733700	0.37473200	-0.69744800
C	-2.10615500	0.74748100	-1.39671300
C	-1.28850900	1.74325500	-0.90599300
C	-1.70240500	2.58785200	0.12583700
C	-2.97771300	2.36031200	0.67763500
C	-3.70546100	1.21837500	0.32768700
O	-0.83815600	3.53080300	0.57734000
C	0.47289500	-0.14888400	-0.49627100
C	1.86127100	0.12852800	0.01952800
N	2.79939100	0.46105300	-0.88888500
O	2.08443400	0.08574900	1.23969900
C	4.15585300	0.86619800	-0.50198400
H	-2.02060700	-4.05562100	-0.40541300
H	-2.82168700	-3.27679500	0.84298000
H	-1.74911100	-2.01521000	-1.53151300
H	-4.07079700	-1.37500200	-1.75225900
H	-4.32599400	-1.34827100	0.00599900
H	0.13674300	-0.62168700	1.45149700

H	-1.72733800	0.10586500	-2.18921700
H	-3.61404600	-3.63258200	-0.62805900
H	-3.34960800	3.01741700	1.46064800
H	-4.59523500	0.96597800	0.89752600
H	-1.21091700	4.01643700	1.32699000
H	0.41184200	-0.62936100	-1.47340400
H	-0.08056100	1.06123000	-0.78846900
H	2.57920300	0.42848800	-1.87503100
H	4.62389100	1.35103300	-1.35711000
H	4.08559100	1.58246400	0.32368100
C	5.04401300	-0.32757700	-0.09273000
O	6.02353600	-0.64070400	-0.72195400
H	3.84125200	-0.60442300	1.39112900
O	4.65585800	-0.99302200	1.00972400

TS<sub>[Yg•GG]→[YGGα•]</sub>

N	-3.28698300	0.67136500	1.54107200
C	-3.23814700	-0.20897400	0.31181800
C	-2.12928000	-1.24276800	0.68372900
C	-2.97648000	0.66634200	-0.94923200
N	-1.80198800	-2.18722500	-0.20959900
O	-1.61731300	-1.15377900	1.80805700
C	-1.66328900	1.41063000	-0.84961500
C	-0.47746800	0.74054700	-1.19484700
C	0.74116300	1.29790100	-0.87816400
C	0.88652500	2.54058000	-0.26180800
C	-0.29741100	3.26066700	-0.00643200
C	-1.54655300	2.69353600	-0.28012200
O	2.06678300	3.08525900	0.09424500
C	-0.62609400	-3.05591900	-0.02227300
C	0.56142700	-2.38871300	-0.73850200
N	1.48434000	-1.76438700	0.05351900
O	0.58634100	-2.33766100	-1.96256500
C	2.39781700	-0.80871700	-0.49436700
C	3.42816600	-0.26745800	0.45417800
O	3.98806100	0.79600500	0.26589500
O	3.62917300	-1.03504200	1.53978900
H	-2.79624900	1.55966200	1.35233200

H	-2.70727000	0.14742200	2.24706800
H	-4.20217500	-0.72156500	0.23393400
H	-2.99430300	0.01059200	-1.82627400
H	-3.82771400	1.34808200	-1.06543600
H	-2.20434300	-2.16473400	-1.13844400
H	-0.51378100	-0.21515200	-1.70700000
H	-4.23125600	0.85864700	1.88146600
H	-0.21712200	4.25692900	0.41810700
H	-2.43837900	3.28961200	-0.08646000
H	4.29586700	-0.60226100	2.10376100
H	-0.47674500	-3.20052500	1.04797500
H	-0.82609600	-4.01720200	-0.49751100
H	1.36961200	-1.78995500	1.05897000
H	2.83285500	-1.14077300	-1.44005700
H	1.77634500	0.20730200	-0.81219800
H	2.80655400	2.47146100	-0.07471300

TS<sub>[YGGa\*]<sub>+</sub>→[YO•GG]<sub>+</sub></sub>

N	4.94486700	-0.72847100	-0.14012800
C	3.62153100	-0.17929600	0.36215200
C	2.61275700	-1.26517500	-0.08245500
C	3.35520300	1.19252400	-0.33180300
N	1.50647800	-1.39025600	0.64931400
O	2.89243400	-1.90773500	-1.10398700
C	1.89759500	1.59571600	-0.28395100
C	1.32612200	2.13002900	0.88670800
C	-0.04759900	2.31543500	0.98527900
C	-0.89079000	1.97634500	-0.09974600
C	-0.30403400	1.53285200	-1.30867000
C	1.07142900	1.33973100	-1.39055600
O	-2.21531500	2.08030000	0.01418200
C	0.29852800	-2.08416600	0.20235100
C	-0.86783300	-1.32406400	0.84859600
N	-1.98992000	-1.13671200	0.08619800
O	-0.75253900	-0.88723200	1.98691200
C	-3.08107200	-0.36106400	0.52189100
C	-4.34703700	-0.50529600	-0.24107200
O	-5.43044300	-0.16712200	0.17497100

O	-4.13377400	-1.02141900	-1.48317500
H	5.60052900	0.00346500	-0.42605700
H	4.65211500	-1.31593200	-0.96115600
H	3.67765200	-0.07389100	1.44780000
H	3.99407600	1.94296700	0.14941400
H	3.66747600	1.10659100	-1.37978800
H	1.36471200	-0.81589800	1.47744100
H	1.95911000	2.38425400	1.73434700
H	5.41038200	-1.33864400	0.53819700
H	-0.94955200	1.33908300	-2.15977100
H	1.50529300	0.97083000	-2.31661200
H	-4.98914700	-1.06009800	-1.94501700
H	0.26873300	-2.09020700	-0.88967200
H	0.29074400	-3.12248800	0.55520400
H	-2.01644500	-1.47344400	-0.87030300
H	-3.19010300	-0.30607900	1.60248200
H	-0.50084300	2.69364000	1.89536600
H	-2.72639600	0.98814900	0.25688100

[Y<sup>o</sup>•GG]<sup>+</sup>

N	0.13019300	-0.77520000	-1.37169900
C	0.19863300	-1.42619200	-0.00845900
C	1.28856400	-2.51059200	-0.16334400
O	1.07702200	-3.41309500	-0.96331500
H	-0.62252800	-0.08035600	-1.41237100
H	-0.01637800	-1.49782000	-2.08679300
H	0.45527700	-0.61994800	0.67860300
C	-1.16023400	-2.05200800	0.37253900
C	-2.29875600	-1.05678000	0.33236100
H	-1.04539700	-2.46319800	1.38222400
H	-1.35113200	-2.89804400	-0.29459800
C	-4.38111600	0.88788200	0.19687000
C	-3.19480200	-1.04358800	-0.76492500
C	-2.46515300	-0.11101300	1.37578200
C	-3.46799300	0.83228800	1.32619700
C	-4.20842900	-0.10834100	-0.84564100
H	-3.09804700	-1.80027300	-1.54103100
H	-1.79731800	-0.14159100	2.23390400

H	-3.61340700	1.55777500	2.12009200
H	-4.90787900	-0.09061600	-1.67532800
O	-5.28193100	1.76221600	0.12496500
N	2.41980900	-2.42656500	0.59032100
C	2.92933000	-1.23099500	1.23597700
C	2.98248600	-0.01857900	0.28174700
O	2.77100600	-0.13722000	-0.92968300
H	3.08924400	-3.15537900	0.36727700
H	2.33705700	-0.97288000	2.12259700
H	3.93930800	-1.45152000	1.59389900
N	3.23214300	1.17543500	0.85885400
C	3.13364100	2.41421900	0.10984200
C	1.69483700	2.73634800	-0.29462300
O	0.75090100	1.97379200	-0.19974700
O	1.61857100	3.97137600	-0.79634600
H	3.35138100	1.23020600	1.86169700
H	3.53719000	3.23473500	0.70635900
H	3.72909200	2.35235100	-0.80729800
H	1.04579000	-0.31133300	-1.53770600
H	0.70213500	4.15975600	-1.06679200