

## **Keto-enol Tautomerism of $\beta$ -diketo Molecules in the Presence of Graphitic Materials Through $\pi$ - $\pi$ Stacking**

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## Synthesis and XPS analysis of GO and P-Gc

GO was synthesized using Hummer's method.<sup>1</sup> 10 g Graphite powder and 5 g NaNO<sub>3</sub> was stirred in 230 ml concentrated H<sub>2</sub>SO<sub>4</sub> which was previously cooled. 30 g KMnO<sub>4</sub> powder was added to the suspension by portion and the temperature was maintained at ~20°C with ice flakes. After KMnO<sub>4</sub> addition was over, ice-flakes were removed and the temperature was elevated to 35°C and the stirring was continued for 30 mins leading the suspension to a thick paste. 450 ml water was added to it very slowly and the effervescence appeared, elevating the temperature of the reaction mixture. It was further heated at 98°C for 15 mins. The resultant brown solution was further diluted with warm water and 3% H<sub>2</sub>O<sub>2</sub> was added slowly, with rigorous stirring, until the suspension turned yellow-brown. After that it was cooled, filtered, and the residue was washed repeatedly with water and dried in oven to get brown powdered solid.

PGc was synthesized following our previous work.<sup>2</sup> 50% (w/v) aqueous solution of phytic acid was irradiated in multimodal scientific microwave oven (model: RG 31L, input voltage: 220 to 240 V, input frequency: 50 Hz, output frequency: 2450 MHz) for 40 seconds in 450 W power. The produced black charred material was cooled, washed repeatedly with water and dried in oven. Then it was grounded to dust using mortar and pestle, sonicated in water for 15 minutes, filtered using a G3 sintered glass crucible and finally the powdered material was dried in oven for overnight.

X-Ray photoelectron spectroscopy (XPS) measurements of GO and PGc were performed in ESCA, Omicron Nanotechnology, Oxford. The binding energies (BE) were calculated using the maximum intensity of the C 1s signal at 284.8 eV as the reference. The atomic percentages of the elements were calculated from the relative intensities of the peaks and considering the relative sensitivity factor (R.S.F.) of C as '1'. Deconvolution of the XP spectrum was done using XPS-Peak software using Gaussian peak shape followed by unbiased curve-fitting. Figures 4a and 4b show the deconvoluted C and O spectra of GO. Contribution of the different functional groups, obtained from the peak areas, are listed in Table S1. The same analysis on PGc was already reported in our previous work.<sup>2</sup> The derived results are presented here again in Table S2.

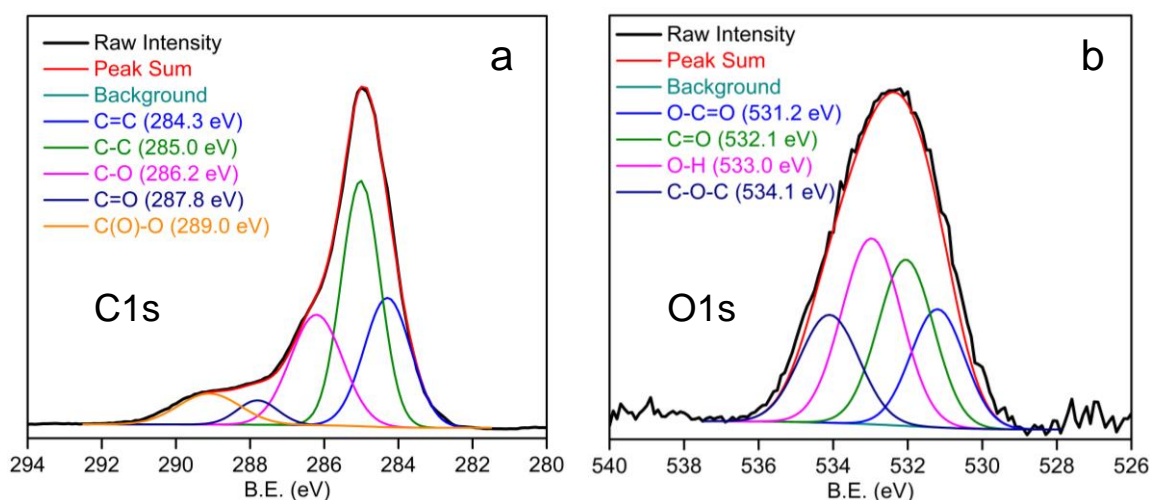


Fig. S1. Deconvolution of XP spectrum of (a) C1s and (b) O1s in GO.

Table S1. Quantification from XPS analysis: Atomic percentages and relative contribution of different functional groups in GO<sup>3</sup>

Atomic %		C functionalities		O functionalities	
Atom	%	Funct. group	Contribution	Funct. group	Contribution
C	72.38	C=C	20.69%	O-C=O	24.76%
		C-C	32.44%	C=O	25.12%
		C-O	22.06%	O-H	25.36%
O	27.62	C=O	11.37%	C-O-C	24.76%
		C(O)-O	13.44%		

Table S2. Quantification from XPS analysis: Atomic percentages and relative contribution of different functional groups in PGc. Data extracted from our previous work.<sup>2</sup>

Atomic %		C functionalities		O functionalities		P functionalities	
Atm.	%	Funct. Gr.	Contribution	Funct. Gr.	Contribution	Funct. Gr.	Contribution
C	83.30	C=C	46.32%	Quinone	11.31%	(Ar) <sub>3</sub> P(O)	26%
O	13.51	C-P, C-C	11.10%	C=O, P=O	26.31%	(Ar) <sub>2</sub> P(O)OH	53%
P	3.18	C-OH	16.50%	C-O, P-O-C	41.08%	COP(O)(OH) <sub>2</sub>	51%
		C=O	13.71%	C-OH, P-OH	18.30%		
		COOH	12.31%	COOH	3.00%		

Table S3. Energy values of the optimized structure

	AA		CF <sub>3</sub> _DK		MAA		DMM	
	E <sub>keto/enol</sub>	E <sub>keto</sub> - E <sub>enol</sub>	E <sub>keto/enol</sub>	E <sub>keto</sub> - E <sub>enol</sub>	E <sub>keto/enol</sub>	E <sub>keto</sub> - E <sub>enol</sub>	E <sub>keto/enol</sub>	E <sub>keto</sub> - E <sub>enol</sub>
Isolated molecules	Keto	-69.998	-72.803	0.499	-75.000	0.631	-80.626	-0.126
	Enol	-70.396	-73.302		-75.631		-80.500	
Stacked on P-Gc	Keto	-680.210	-683.500	§	-685.553	0.074	-690.785	-0.054
	Enol	-680.720	-683.505		-685.627		-690.731	
Stacked on GO (above)	Keto	-989.242	-994.609	0.377	-997.104	0.078	-1002.455	-0.050
	Enol	-989.499	-994.986		-997.182		-1002.405	
Stacked on GO (below)	Keto	-988.864	-994.376	0.528	-996.603	0.667	-1002.231	-0.046
	Enol	-989.392	-994.904		-997.270		-1002.185	
Stacked on G	Keto	-845.263	-848.145	0.503	-850.400	0.640	-856.028	-0.077
	enol	-845.766	-848.648		-851.040		-855.951	

§both keto and enol resulted in the enol form after stacking, so the “difference” between keto and enol cannot be calculated here

For each of the four diketo molecules, E<sub>keto</sub> - E<sub>enol</sub> energy was calculated and listed in each of the columns. It was a measurement of the relative stability of enol structures, in isolated and stacked condition. Except DMM, the other three diketo molecules were more stable in enol form. This enol-stability was observed increasing after stacking on P-Gc, G, and the ‘below’ side of GO, whereas for the ‘above’ side of GO this stability decreased. For the two esters, MAA and DMM, the E<sub>keto</sub> - E<sub>enol</sub> stabilization energy decreased in case of P-Gc too. It is clear from this comparison between isolated and stacked that, **stabilization of enol** is majorly controlled by  $\pi$ - $\pi$  stacking while we had discussed earlier from Table 1 (main manuscript) that **enolization** is mainly controlled by the effect of both graphitic  $\pi$ -cloud and acid containing functional groups.

Figures: GO and diketo molecules

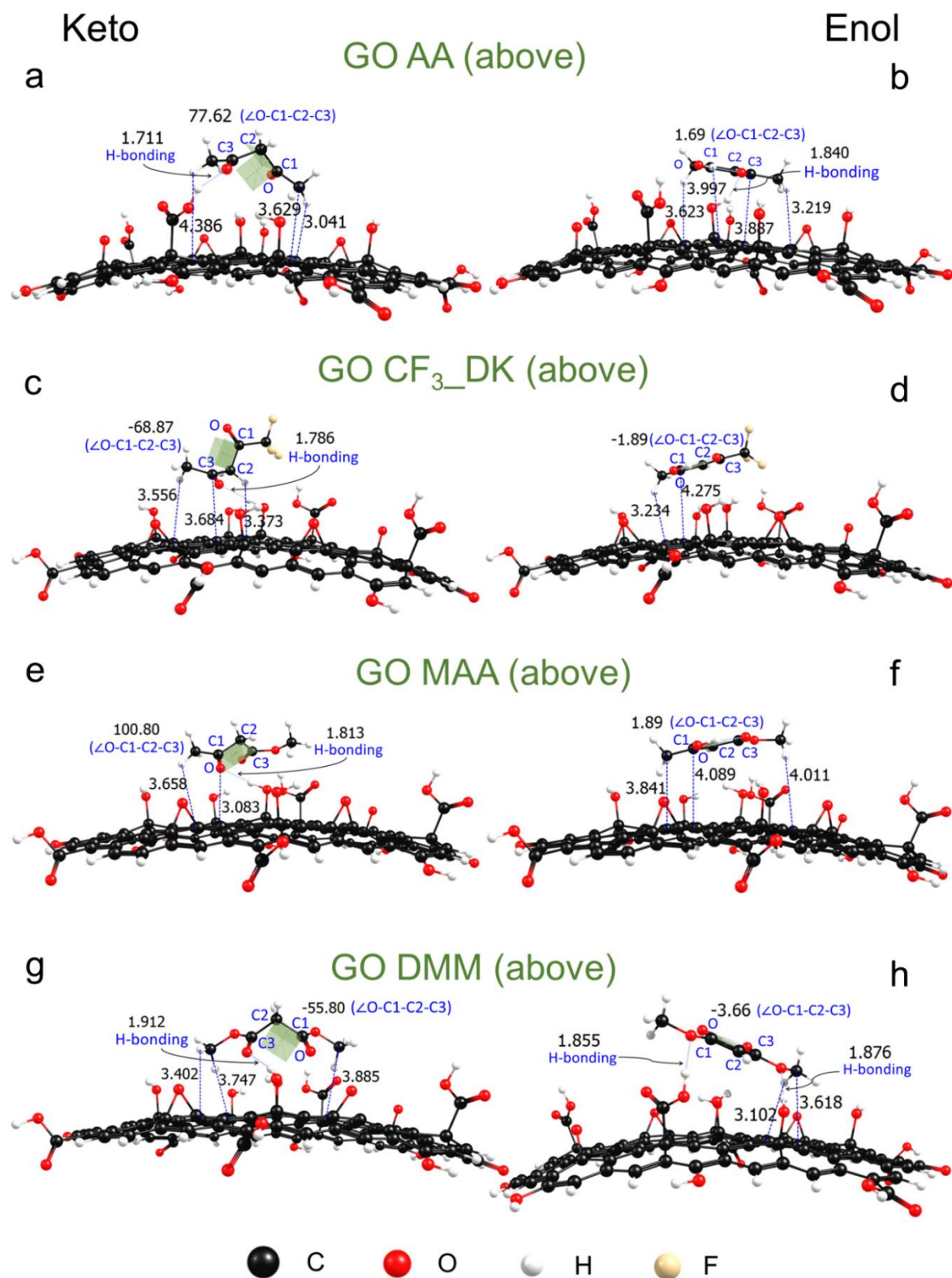


Fig. S2. The interaction of  $\beta$ -diketo molecules at the 'above' side of GO surface. Weak bonds are shown with dotted lines along with their bond lengths in Å. The dihedral angles are given in  $^{\circ}$ .

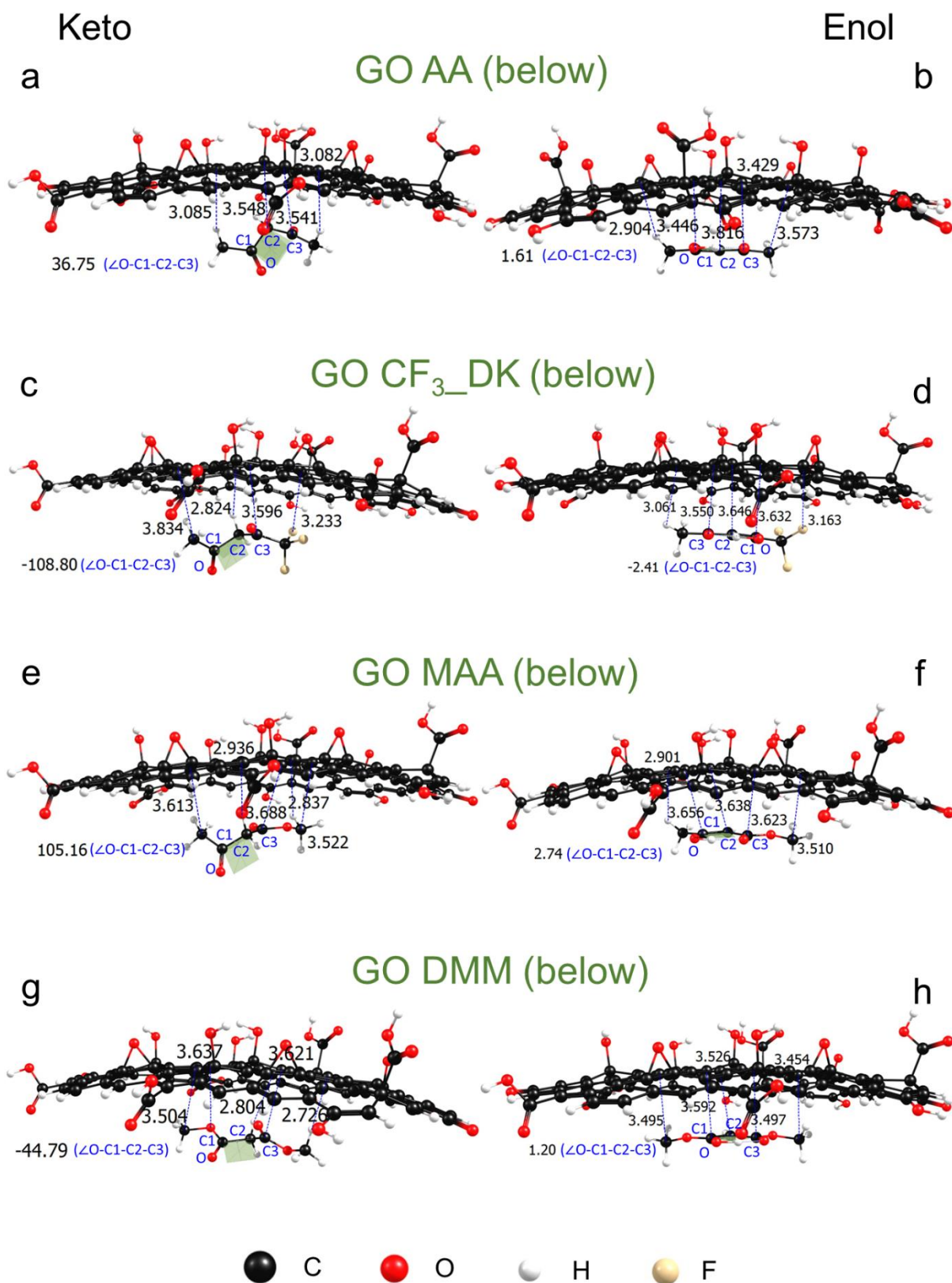


Fig. S3. The interaction of  $\beta$ -diketo molecules at the ‘below’ side of GO surface. Other details are the same as in Fig. S2.



Figures: G and diketo molecules

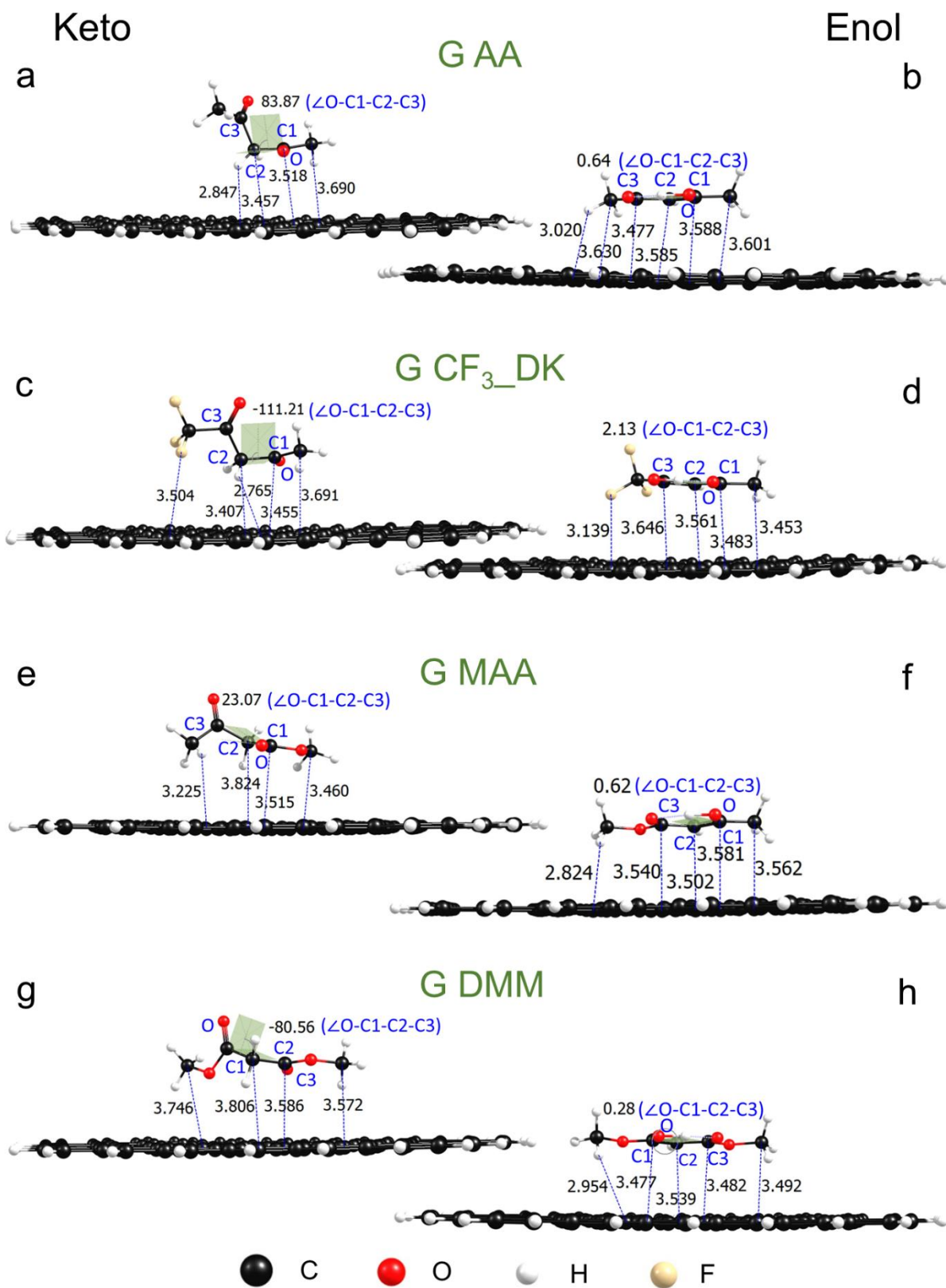


Fig S4. The interaction of  $\beta$ -diketo molecules over G surface. Other details are the same as in Fig. S2.



Cartesian coordinates of the optimized geometries:

PGc-AA-keto							
C	6.367886	11.253309	9.565232	C	3.169616	14.990115	10.656302
C	6.541238	12.673401	9.930806	C	2.629158	11.110344	8.818461
C	7.863398	13.316428	9.961861	C	1.813629	13.165395	9.839822
C	9.088773	12.577882	9.966525	C	1.698801	12.137534	9.213548
C	7.489424	10.366164	9.487946	C	7.481520	6.307173	12.478352
C	10.286533	10.148995	9.348508	C	8.947648	5.923378	12.289345
C	7.446423	9.070210	8.889467	C	9.987770	6.809681	12.480047
C	10.395791	13.145838	9.802313	C	11.405882	6.517437	12.339936
C	11.551917	10.840503	9.342461	C	12.432961	7.634370	12.602937
C	11.615973	12.290319	9.698119	O	14.460912	11.427679	11.498646
C	4.955699	9.057939	9.168640	O	9.021352	10.481648	11.959656
C	5.042029	10.722025	9.215620	O	15.454699	12.688649	9.660517
C	12.717331	10.081711	8.863399	O	2.655154	8.679532	9.989230
C	12.510170	8.761693	8.263744	O	1.041454	7.720386	11.532251
C	8.085867	14.736424	9.884372	O	0.326888	7.938009	8.886196
C	10.504013	14.608196	9.742486	O	0.925761	9.598412	10.488065
C	9.239608	15.289968	9.765878	O	11.006971	2.992470	8.521711
C	5.338681	13.437676	10.066625	O	10.865243	2.702734	6.276771
C	4.104430	12.881713	9.826121	O	5.771786	3.475542	6.955390
C	3.914406	11.599088	9.396005	O	3.580854	4.814439	7.078803
C	12.891027	12.972262	9.821194	O	14.196661	15.030643	9.913842
C	11.810401	15.175187	9.715981	O	16.745164	6.142596	5.865919
C	12.914738	14.382512	9.812850	O	9.327609	4.802304	11.924756
C	14.079601	10.571505	9.006845	O	11.805598	5.395986	12.015390
C	15.126552	9.801730	8.465455	P	8.980842	10.835931	10.370271
C	14.944286	8.605209	7.845956	P	14.464763	12.072953	9.945025
C	13.665514	8.002199	7.726679	P	1.293981	8.523654	10.101660
C	13.495367	6.786429	7.176970	P	10.773649	3.685871	6.958717
C	10.040515	8.873976	8.730278	H	14.779573	12.145582	12.096549
C	8.675906	8.318443	8.588497	H	0.442342	7.654785	12.068629
C	6.119362	8.548258	8.528226	H	0.083768	8.266729	8.255830
C	6.082330	7.216387	8.004146	H	11.104628	2.196252	8.524686
C	7.205255	6.497583	7.775124	H	14.066765	15.987947	9.903609
C	11.187825	8.167141	8.189081	H	15.020923	4.334800	5.843581
C	11.002835	6.832919	7.599193	H	12.916581	3.410746	5.602174
C	12.165053	6.174566	7.100751	H	8.213694	3.413828	6.840253
C	9.695131	6.302539	7.559103	H	2.844483	6.909095	8.307234
C	8.532401	6.987850	7.978367	H	0.937452	13.782343	9.974317
C	6.853635	15.657921	9.947989	H	2.293108	15.495279	11.034379
C	5.429948	15.055116	10.285330	H	4.433476	16.569892	11.315034
C	4.801151	6.701918	8.102611	H	9.260620	16.365986	9.675636
C	3.865394	7.424047	8.637275	H	11.926998	16.244404	9.618099
C	3.716931	8.637720	9.241195	H	16.133370	10.183929	8.546953
C	12.032250	4.906898	6.521630	H	16.876906	7.982825	8.071067
C	9.538467	5.001074	7.067527	H	0.718839	11.963462	8.794294
C	7.057603	5.186128	7.307915	H	2.416902	10.336001	8.221971
C	4.681284	5.346772	7.339906	H	6.961217	16.716373	9.762229
C	8.293996	4.468949	7.056291	H	17.232583	6.880230	5.476399
C	5.849478	4.697522	7.206845	H	6.906097	5.441636	12.793435
C	13.013257	4.368941	6.090964	H	7.381014	7.082752	13.230455
C	14.400211	6.112652	6.712658	H	7.048019	6.675336	11.550573

C	14.171620	4.901363	6.195845	H	12.452143	7.917639	13.661473
C	15.696576	6.663996	6.703897	H	13.445533	7.318283	12.327449
C	5.912509	7.817145	7.614023	H	12.199566	8.535392	12.024323
C	2.972779	13.679083	10.034849	H	9.651141	7.397696	13.249559
C	4.364015	15.624718	10.797132	H	10.291617	7.385267	11.804690
PGc-AA-enol							
C	11.286583	13.168193	9.758833	C	8.198217	17.263678	10.048506
C	11.485813	14.544072	10.183412	C	7.837145	13.414479	8.298114
C	12.787674	15.084868	10.500522	C	6.899687	15.589360	8.774054
C	13.967487	14.318224	10.432099	C	6.821603	14.348664	8.140344
C	12.372978	12.244615	9.689796	C	13.842557	7.191034	11.286096
C	15.105626	12.023553	9.445657	C	15.243647	7.728233	11.241009
C	12.309825	11.014781	9.032582	C	15.548208	8.999569	11.788487
C	15.263483	14.852491	10.439699	C	16.850071	9.486063	11.775864
C	16.326431	12.707420	9.431907	C	17.239380	10.801443	12.352920
C	16.435858	14.076882	10.038136	O	19.721237	15.113918	8.375024
C	9.851658	11.303791	9.110820	O	13.953728	12.004610	11.935545
C	10.013290	12.722001	9.334890	O	20.186447	13.772435	10.578075
C	17.437576	12.009216	8.809539	O	7.643627	11.284086	10.012803
C	17.248606	10.687674	8.274418	O	6.192834	9.527263	10.967831
C	12.931816	16.480032	10.830681	O	5.504491	10.579250	8.803857
C	15.383965	16.238005	10.821868	O	5.395509	12.031615	10.959071
C	14.222702	16.994513	11.038107	O	15.781741	5.063241	8.960619
C	10.377593	15.426255	10.169291	O	15.358828	4.394198	6.531610
C	9.124766	15.010053	9.612526	O	10.367566	5.372638	6.773773
C	8.965152	13.688792	9.100117	O	8.194023	6.684584	7.911413
C	17.663935	14.740718	10.158243	O	19.057268	16.456314	11.005254
C	16.669594	16.798080	11.029900	O	21.599659	7.994035	5.894754
C	17.773109	16.035707	10.757507	O	16.168186	7.003175	10.713440
C	19.792864	11.909609	8.118792	O	17.840485	8.779872	11.247348
C	19.630411	10.627776	7.575512	P	13.855259	12.579973	10.554783
C	18.354309	9.998404	7.686704	P	19.171970	14.164309	9.374908
C	18.219656	8.655685	7.225283	P	6.095150	10.952553	10.253844
C	14.840206	10.764362	8.810424	P	15.575559	5.534654	7.451228
C	13.508845	10.242674	8.696055	H	20.519852	14.588327	11.003490
C	10.995467	10.496856	8.785639	H	5.375791	9.293145	11.446065
C	10.839958	9.154958	8.362334	H	4.980676	11.323850	8.452976
C	12.017107	8.369222	8.027770	H	15.912222	5.789937	9.656964
C	15.962350	10.032450	8.293655	H	19.064888	17.407339	11.217131
C	15.810811	8.687916	7.855598	H	20.108027	6.154142	5.787477
C	16.981781	7.956953	7.382613	H	17.987535	4.888272	6.215983
C	14.485554	8.113594	7.849111	H	12.837353	5.211319	7.018998
C	13.337433	8.923810	8.174608	H	7.504345	8.786433	8.963114
C	11.779245	17.291397	10.929840	H	6.085001	16.310787	8.681155
C	10.525978	16.802397	10.597486	H	7.344449	17.943621	10.001722
C	9.544876	8.596853	8.348032	H	9.495895	18.683081	10.974735
C	8.455859	9.310034	8.869873	H	14.327758	18.037806	11.348138
C	8.617997	10.613139	9.293880	H	16.764380	17.818701	11.411144
C	18.744034	12.563208	8.735479	H	20.770672	12.394593	8.061113
C	16.971104	6.579018	7.056541	H	21.679129	10.497180	6.873661
C	14.255890	6.746164	7.509389	H	5.959508	14.112927	7.512753
C	11.857572	7.051471	7.563112	H	7.773007	12.459679	7.775576
C	9.300243	7.218689	7.881978	H	11.889278	18.341146	11.214623

C	12.980659	6.249277	7.328892	H	22.394989	8.556167	5.851822
C	10.522757	6.447637	7.344383	H	13.757574	6.496538	12.138012
C	18.076180	5.944305	6.479684	H	14.758971	9.633574	12.190446
C	19.344761	7.983627	6.644107	H	13.104032	7.991272	11.420614
C	19.248180	6.640761	6.246386	H	13.619104	6.616944	10.376668
C	20.588036	8.689072	6.493430	H	17.393061	7.905689	10.916286
C	20.725130	9.968996	6.956524	H	17.748985	10.636421	13.316587
C	8.052250	15.948747	9.485083	H	17.958855	11.306043	11.692141
C	9.378691	17.669373	10.585186	H	16.356676	11.432635	12.516351
PGc-CF <sub>3</sub> _DK-keto							
C	11.218298	16.118977	9.738101	C	8.192074	20.254572	10.082857
C	11.425579	17.471577	10.228559	C	7.836159	16.488371	8.157880
C	12.725412	17.976852	10.608109	C	6.918303	18.659389	8.686993
C	13.898579	17.198940	10.531224	C	6.844968	17.448093	7.998242
C	12.291082	15.181921	9.664500	C	13.958496	11.170177	11.604461
C	15.021217	14.939380	9.456726	C	15.439205	11.260212	11.420719
C	12.221969	13.970023	8.975922	C	16.146746	12.420288	11.879965
C	15.199396	17.724348	10.548886	C	17.514332	12.449744	11.755035
C	16.243074	15.619342	9.444180	C	18.359528	13.605654	12.278027
C	16.362059	16.970322	10.083018	O	19.005630	19.357208	10.978036
C	9.770136	14.302767	8.981125	O	7.526015	14.310758	9.793105
C	9.953198	15.711156	9.253355	O	13.816439	14.793557	11.913860
C	17.344595	14.931829	8.788895	O	20.203833	16.815735	10.311289
C	17.155802	13.600893	8.278876	O	19.407423	18.110949	8.176708
C	12.879885	19.355690	10.995826	O	5.940659	12.589605	10.592714
C	15.329319	19.095253	10.978405	O	5.452914	13.728661	8.419310
C	14.174172	19.848032	11.235365	O	5.248147	15.123756	10.606574
C	10.332945	18.373024	10.212489	O	15.646376	8.141192	9.262923
C	9.096399	18.003639	9.589663	O	15.287714	7.202266	6.915135
C	8.934196	16.707779	9.016086	O	10.276302	8.317081	6.737958
C	17.588823	17.642611	10.161673	O	8.075931	9.718859	7.686572
C	16.619825	19.652828	11.162292	O	21.482395	10.851906	5.925941
C	17.715307	18.917202	10.798981	O	16.080740	10.295012	10.879171
C	18.639006	15.502411	8.654613	O	18.228889	11.477323	11.221855
C	19.677464	14.843687	8.024761	P	19.041010	17.134684	9.233834
C	19.520832	13.538713	7.533904	P	13.762082	15.459752	10.571012
C	18.254499	12.901314	7.691977	P	5.952269	14.037039	9.917820
C	18.121637	11.540602	7.283582	P	15.475908	8.443847	7.698069
C	14.749679	13.689701	8.806944	H	20.496008	17.648584	10.734353
C	13.416116	13.183969	8.663708	H	5.095857	12.394939	11.039433
C	10.908527	13.477061	8.682755	H	4.992885	14.507434	8.053432
C	10.745840	12.138412	8.247931	H	15.718597	8.932190	9.868902
C	11.920103	11.324766	7.971170	H	19.007318	20.299343	11.226357
C	15.871063	12.946002	8.313004	H	20.007425	8.980639	5.953248
C	15.716432	11.592846	7.910694	H	17.905182	7.721200	6.479897
C	16.888981	10.843418	7.478992	H	12.732705	8.115412	7.125612
C	14.387825	11.029091	7.894628	H	7.382955	11.832021	8.711630
C	13.241543	11.862000	8.154631	H	6.120952	19.399530	8.591048
C	11.736548	20.179792	11.098452	H	7.353335	20.952406	10.029487
C	10.487437	19.726978	10.703932	H	9.475591	21.609718	11.118864
C	9.442941	11.604565	8.181099	H	14.287061	20.877905	11.584675
C	8.347093	12.338012	8.658323	H	16.723840	20.659998	11.575491
C	8.516348	13.634172	9.102140	H	20.647663	15.336916	7.926255

C	16.879635	9.449820	7.229715	H	21.554796	13.394621	6.791985
C	14.154313	9.650515	7.609270	H	6.005680	17.256908	7.326162
C	11.761255	9.995486	7.538146	H	7.777984	15.556638	7.594282
C	9.194522	10.225321	7.717665	H	11.854311	21.215599	11.427878
C	12.880674	9.164613	7.392282	H	22.271698	11.418388	5.845254
C	10.427131	9.410462	7.273774	H	13.760636	10.691032	12.578619
C	17.985661	8.791481	6.681534	H	15.596992	13.268106	12.288743
C	19.243034	10.848773	6.721116	H	13.501289	12.169244	11.628620
C	19.149603	9.485286	6.396444	H	13.508829	10.541417	10.825527
C	20.475624	11.561128	6.515506	H	17.504814	10.767891	10.957650
C	20.607813	12.862535	6.918988	F	17.619759	14.732909	12.445565
C	8.046453	18.967045	9.459118	F	18.897680	13.280043	13.490649
C	9.356470	20.615116	10.683331	F	19.383244	13.892837	11.437122

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C	11.227505	16.119150	9.815004	C	8.198110	20.240316	10.289736
C	11.448474	17.472528	10.296852	C	7.789629	16.481668	8.360180
C	12.760687	17.984692	10.618837	C	6.882088	18.646978	8.930894
C	13.933088	17.211945	10.491723	C	6.790606	17.438976	8.238257
C	12.299002	15.184130	9.701832	C	14.058372	11.215355	11.613369
C	15.018826	14.947659	9.386492	C	15.532648	11.283513	11.376852
C	12.206743	13.971746	9.016080	C	16.269602	12.443476	11.787988
C	15.230136	17.744783	10.444323	C	17.631397	12.456375	11.608619
C	16.237339	15.630364	9.321351	C	18.508179	13.612607	12.075909
C	16.374899	16.992102	9.933795	O	19.036428	19.428364	10.627123
C	9.756897	14.302027	9.106570	O	7.552450	14.301138	10.012709
C	9.946519	15.708735	9.377844	O	13.919489	14.814918	11.890652
C	17.318750	14.931752	8.644292	O	20.227867	16.890951	9.991184
C	17.119080	13.587475	8.174498	O	19.311850	18.103539	7.855893
C	12.924475	19.365305	10.995485	O	5.967421	12.568418	10.802788
C	15.370953	19.121580	10.852095	O	5.401745	13.825374	8.720130
C	14.225430	19.867731	11.165434	O	5.339700	15.112770	10.982702
C	10.351811	18.368774	10.327663	O	15.589306	8.132517	9.267186
C	9.093366	17.996105	9.752623	O	15.196371	7.179864	6.929813
C	8.915754	16.702057	9.180696	O	10.187413	8.292476	6.895953
C	17.597572	17.676596	9.939110	O	7.999644	9.770545	7.735751
C	16.663010	19.695673	10.954299	O	21.429644	10.743586	5.904809
C	17.744057	18.966686	10.538975	O	16.143209	10.300547	10.831335
C	18.607050	15.501216	8.459042	O	18.314810	11.467273	11.065360
C	19.635912	14.821214	7.837043	P	19.010813	17.157734	8.960035
C	19.474918	13.497305	7.402935	P	13.804585	15.472203	10.547062
C	18.208382	12.868817	7.593231	P	5.981813	14.048922	10.203687
C	18.066996	11.497556	7.225444	P	15.402791	8.425309	7.701955
C	14.727009	13.689592	8.761309	H	20.528814	17.742998	10.367494
C	13.389330	13.184039	8.665219	H	5.145975	12.375966	11.292110
C	10.884322	13.478769	8.765732	H	4.973968	14.642633	8.401782
C	10.704880	12.143035	8.328343	H	15.708944	8.927726	9.860233
C	11.868936	11.325886	8.020443	H	19.039177	20.376488	10.851177
C	15.833897	12.936336	8.249017	H	19.937716	8.894161	5.958636
C	15.666175	11.577086	7.872381	H	17.821867	7.664256	6.500333
C	16.830120	10.813271	7.440229	H	12.649085	8.107265	7.182446
C	14.334416	11.019914	7.889190	H	7.352591	11.844866	8.878458
C	13.196895	11.859359	8.168962	H	6.079309	19.384590	8.865632
C	11.782313	20.182442	11.152707	H	7.354564	20.934196	10.272660

C	10.519465	19.722326	10.815230	H	9.514828	21.596939	11.281104
C	9.397464	11.616773	8.286429	H	14.348925	20.900894	11.501307
C	8.317516	12.346825	8.805061	H	16.778231	20.711205	11.343313
C	8.507366	13.633819	9.266334	H	20.603674	15.311195	7.704566
C	16.810328	9.415761	7.215417	H	21.508280	13.319865	6.667029
C	14.088115	9.639887	7.621059	H	5.931651	17.249943	7.590549
C	11.694794	9.994269	7.600259	H	7.715635	15.552087	7.794733
C	9.128930	10.249194	7.800662	H	11.909041	21.219185	11.475658
C	12.807779	9.158138	7.436137	H	22.223312	11.301652	5.809015
C	10.352709	9.408474	7.378044	H	13.888407	10.739030	12.594184
C	17.911488	8.737369	6.681901	H	15.744472	13.303739	12.203025
C	19.184525	10.784256	6.681631	H	13.616019	12.220661	11.651321
C	19.082306	9.414709	6.387752	H	13.573274	10.591249	10.851925
C	20.423088	11.480723	6.459540	H	17.574194	10.760191	10.843873
C	20.559427	12.795938	6.812838	F	17.786205	14.749056	12.256555
C	8.035209	18.955395	9.664889	F	19.095768	13.300528	13.269004
C	9.383489	20.603865	10.845659	F	19.497128	13.877614	11.187195

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C	9.299593	14.172739	9.728807	C	5.923559	14.562222	8.138636
C	9.516057	15.525636	10.214864	C	5.022542	16.742943	8.656111
C	10.817863	16.020868	10.601473	C	4.940909	15.529485	7.972083
C	11.982875	15.230170	10.542583	C	13.100510	9.023898	11.548699
C	10.364948	13.226644	9.664024	C	13.556353	10.117297	12.488073
C	13.096947	12.954858	9.491683	C	15.058162	10.205081	12.607659
C	10.292327	12.015405	8.974440	C	17.032070	11.003347	11.585463
C	13.289495	15.738642	10.586613	C	11.620064	8.762334	11.507826
C	14.326135	13.620483	9.502073	O	18.217138	14.600864	10.596179
C	14.451679	14.964054	10.154773	O	11.861739	12.831333	11.931449
C	7.843845	12.366383	8.962696	O	17.705523	16.062311	8.481684
C	8.033762	13.772930	9.239540	O	5.600710	12.380571	9.773107
C	15.424207	12.934086	8.844276	O	4.018121	10.652655	10.562621
C	15.224387	11.618950	8.301478	O	3.515332	11.820452	8.407505
C	10.983653	17.400244	10.984154	O	3.330826	13.187761	10.613570
C	13.430360	17.107584	11.018246	O	13.694945	6.224070	9.251514
C	12.279811	17.878229	11.243046	O	13.332520	5.236279	6.917295
C	8.431348	16.436007	10.190226	O	8.322310	6.370399	6.722441
C	7.193285	16.073149	9.566586	O	6.113001	7.845501	7.520953
C	7.022030	14.776136	8.997942	O	17.108923	17.265713	11.200571
C	15.688476	15.607983	10.287750	O	19.530449	8.886043	5.894042
C	14.724815	17.637802	11.252369	O	13.907057	8.384506	10.865801
C	15.817769	16.873478	10.943205	O	15.717712	9.681420	13.489630
C	16.726768	13.491556	8.737823	O	15.587120	10.936058	11.594269
C	17.756943	12.847412	8.077040	P	11.828100	13.492465	10.584625
C	17.586819	11.559529	7.546043	P	17.175549	15.062099	9.441288
C	16.317625	10.925135	7.698600	P	4.027446	12.108594	9.905709
C	16.177200	9.571335	7.270456	P	13.523306	6.487696	7.683999
C	12.819581	11.714256	8.828527	H	18.553308	15.388831	11.069440
C	11.482555	11.221370	8.668846	H	3.173752	10.451807	11.007368
C	8.977835	11.534251	8.666511	H	3.062109	12.607828	8.051679
C	8.807503	10.201469	8.216649	H	13.734497	7.037004	9.842210
C	9.977334	9.381184	7.941509	H	17.132391	18.207964	11.447741
C	13.937081	10.971336	8.326764	H	18.044519	7.021518	5.895998
C	13.774833	9.626148	7.904325	H	15.940702	5.763309	6.422117

C	14.942787	8.877414	7.461380	H	10.775885	6.170858	7.085156
C	12.443010	9.071205	7.877106	H	5.436775	9.922300	8.639647
C	11.301099	9.907593	8.141309	H	4.231842	17.489498	8.555438
C	9.847315	18.235802	11.072625	H	5.471498	19.036499	9.992790
C	8.596085	17.791246	10.675329	H	7.597468	19.682819	11.081182
C	7.500048	9.682610	8.124972	H	12.398575	18.907696	11.591837
C	6.406697	10.418603	8.605119	H	14.834647	18.641005	11.673515
C	6.585336	11.705417	9.072091	H	18.730726	13.336483	7.992096
C	14.926551	7.487050	7.196921	H	19.616379	11.417929	6.789300
C	12.203310	7.696585	7.579274	H	4.102522	15.342728	7.297593
C	9.812152	8.055414	7.499786	H	5.859032	13.629052	7.578154
C	7.241832	8.319180	7.622028	H	9.972013	19.272036	11.398335
C	10.928234	7.218379	7.355820	H	20.320524	9.451287	5.812268
C	8.475679	7.478319	7.226845	H	13.132185	9.917519	13.484438
C	16.025892	6.831234	6.633988	H	13.108122	11.075903	12.155186
C	17.293015	8.882401	6.693592	H	17.401871	11.423304	12.530494
C	17.191483	7.524084	6.350737	H	17.453917	9.998241	11.446071
C	18.527769	9.592731	6.493039	H	17.291731	11.656337	10.746665
C	18.667221	10.888683	6.912697	H	11.363327	8.082677	10.686897
C	6.151094	17.044159	9.430018	H	11.312497	8.307229	12.463552
C	7.471663	18.687519	10.649296	H	11.067835	9.710256	11.418531
C	6.305286	18.332926	10.049183				

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C	11.294407	11.125283	10.006198	C	7.910711	11.255235	8.398607
C	11.463097	12.524766	10.362551	C	6.922241	13.433075	8.741778
C	12.749343	13.105085	10.674364	C	6.892306	12.167907	8.154065
C	13.944307	12.359904	10.650976	C	15.428103	6.121850	11.892381
C	12.395285	10.218096	10.012132	C	14.188196	5.401128	11.931440
C	15.129356	10.039161	9.799508	C	13.022765	6.039574	12.278008
C	12.356616	8.946288	9.441739	C	11.701040	5.347998	12.329501
C	15.227464	12.922687	10.625705	C	17.779102	6.012121	11.441927
C	16.325901	10.757337	9.709085	O	18.990456	14.649076	11.008859
C	16.411182	12.158523	10.237164	O	5.318471	10.091502	10.849537
C	9.894820	9.205496	9.436119	O	13.936689	10.142319	12.288505
C	10.039859	10.637786	9.569740	O	20.207891	12.001366	10.580942
C	17.432253	10.072290	9.060026	O	19.553228	13.247604	8.370777
C	17.266630	8.723605	8.592571	O	7.640087	9.227967	10.231148
C	12.862526	14.516491	10.940130	O	6.004250	7.564006	11.057442
C	15.319237	14.327438	10.940027	O	5.646517	8.540121	8.786015
C	14.142282	15.066695	11.129149	O	16.170626	3.185622	9.788607
C	10.342217	13.385962	10.278567	O	15.591973	2.219059	7.503392
C	9.115608	12.924583	9.699195	O	10.581722	2.977372	8.012125
C	8.994458	11.579647	9.241048	O	8.328214	4.479855	8.574358
C	17.621550	12.862070	10.280246	O	21.513359	6.121638	5.939250
C	16.595068	14.926505	11.097670	O	15.593807	7.312750	12.184663
C	17.711166	14.183598	10.822334	O	12.944588	7.332462	12.593331
C	18.705048	10.674669	8.868591	O	16.495285	5.344642	11.464466
C	19.728376	10.045269	8.184808	P	6.060914	8.960592	10.283136
C	19.582909	8.736779	7.700913	P	13.863259	10.629874	10.877632
C	18.354824	8.054926	7.949840	P	19.106480	12.312675	9.434196
C	18.248808	6.684604	7.565966	P	15.802668	3.478422	8.251301
C	14.887449	8.743407	9.235271	H	20.510509	12.841884	10.980874

C	13.571808	8.178296	9.168274	H	5.129400	7.397035	11.454964
C	11.056868	8.387415	9.216376	H	5.229569	9.295707	8.330763
C	10.934525	7.007288	8.920702	H	16.270916	3.981485	10.378190
C	12.131216	6.212904	8.687584	H	18.977482	15.607707	11.182622
C	16.013086	8.021317	8.720466	H	20.125492	4.191849	6.099296
C	15.896402	6.647506	8.375245	H	18.132820	2.850424	6.817456
C	17.066235	5.939656	7.868819	H	13.047706	2.982474	8.059978
C	14.602060	6.020671	8.482014	H	7.581680	6.651691	9.424772
C	13.434334	6.817352	8.761417	H	6.102111	14.136564	8.582826
C	11.693012	15.308535	10.985665	H	7.278083	15.840939	9.898800
C	10.456038	14.782052	10.647638	H	9.382091	16.657129	10.914774
C	9.649014	6.428864	8.920601	H	14.224670	16.125132	11.390618
C	8.531256	7.176120	9.318825	H	16.672247	15.964408	11.433378
C	8.659529	8.516889	9.620315	H	20.673031	10.572016	8.026778
C	17.101099	4.543019	7.638107	H	21.557703	8.668139	6.802926
C	14.420464	4.617247	8.295735	H	6.064730	11.897733	7.494384
C	12.012444	4.840230	8.400718	H	7.887168	10.277725	7.915363
C	9.438963	5.004134	8.599984	H	11.778289	16.372026	11.224442
C	13.161464	4.054729	8.236555	H	22.267555	6.720339	5.787228
C	10.698791	4.164410	8.301691	H	14.166469	4.345319	11.670874
C	18.184023	3.925722	7.001760	H	13.851709	7.757933	12.539245
C	19.349972	6.033624	6.919453	H	11.777257	4.306372	11.996929
C	19.288038	4.664264	6.611586	H	11.307691	5.373104	13.357351
C	20.531378	6.793828	6.610661	H	10.976176	5.883089	11.697122
C	20.645315	8.099595	7.004373	H	17.729681	6.923630	10.832163
C	8.036314	13.839655	9.488387	H	18.082705	6.277035	12.463377
C	9.294725	15.626375	10.563841	H	18.475174	5.288034	11.003965
C	8.140406	15.178448	10.003658				

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C	6.367886	11.253309	9.565232	C	2.629158	11.110344	8.818461
C	6.541238	12.673401	9.930806	C	1.813629	13.165395	9.839822
C	7.863398	13.316428	9.961861	C	1.698801	12.137534	9.213548
C	9.088773	12.577882	9.966525	C	8.947648	5.923378	12.289345
C	7.489424	10.366164	9.487946	C	9.987770	6.809681	12.480047
C	10.286533	10.148995	9.348508	C	11.405882	6.517437	12.339936
C	7.446423	9.070210	8.889467	C	13.691219	7.187283	12.925136
C	10.395791	13.145838	9.802313	C	6.625861	5.211769	12.631163
C	11.551917	10.840503	9.342461	O	14.460912	11.427679	11.498646
C	11.615973	12.290319	9.698119	O	9.021352	10.481648	11.959656
C	4.955699	9.057939	9.168640	O	15.454699	12.688649	9.660517
C	5.042029	10.722025	9.215620	O	2.655154	8.679532	9.989230
C	12.717331	10.081711	8.863399	O	1.041454	7.720386	11.532251
C	12.510170	8.761693	8.263744	O	0.326888	7.938009	8.886196
C	8.085867	14.736424	9.884372	O	0.925761	9.598412	10.488065
C	10.504013	14.608196	9.742486	O	11.006971	2.992470	8.521711
C	9.239608	15.289968	9.765878	O	10.865243	2.702734	6.276771
C	5.338681	13.437676	10.066625	O	5.771786	3.475542	6.955390
C	4.104430	12.881713	9.826121	O	3.580854	4.814439	7.078803
C	3.914406	11.599088	9.396005	O	14.196661	15.030643	9.913842
C	12.891027	12.972262	9.821194	O	16.745164	6.142596	5.865919
C	11.810401	15.175187	9.715981	O	9.327609	4.802304	11.924756
C	12.914738	14.382512	9.812850	O	11.805598	5.395986	12.015390
C	14.079601	10.571505	9.006845	O	12.366267	7.561842	12.585859



C	15.126552	9.801730	8.465455	O	7.563962	6.266185	12.493054
C	14.944286	8.605209	7.845956	P	8.980842	10.835931	10.370271
C	13.665514	8.002199	7.726679	P	14.464763	12.072953	9.945025
C	13.495367	6.786429	7.176970	P	1.293981	8.523654	10.101660
C	10.040515	8.873976	8.730278	P	10.773649	3.685871	6.958717
C	8.675906	8.318443	8.588497	H	14.779573	12.145582	12.096549
C	6.119362	8.548258	8.528226	H	0.442342	7.654785	12.068629
C	6.082330	7.216387	8.004146	H	0.083768	8.266729	8.255830
C	7.205255	6.497583	7.775124	H	11.104628	2.196252	8.524686
C	11.187825	8.167141	8.189081	H	14.066765	15.987947	9.903609
C	11.002835	6.832919	7.599193	H	15.020923	4.334800	5.843581
C	12.165053	6.174566	7.100751	H	12.916581	3.410746	5.602174
C	9.695131	6.302539	7.559103	H	8.213694	3.413828	6.840253
C	8.532401	6.987850	7.978367	H	2.844483	6.909095	8.307234
C	6.853635	15.657921	9.947989	H	0.937452	13.782343	9.974317
C	5.429948	15.055116	10.285330	H	2.293108	15.495279	11.034379
C	4.801151	6.701918	8.102611	H	4.433476	16.569892	11.315034
C	3.865394	7.424047	8.637275	H	9.260620	16.365986	9.675636
C	3.716931	8.637720	9.241195	H	11.926998	16.244404	9.618099
C	12.032250	4.906898	6.521630	H	16.133370	10.183929	8.546953
C	9.538467	5.001074	7.067527	H	16.876906	7.982825	8.071067
C	7.057603	5.186128	7.307915	H	0.718839	11.963462	8.794294
C	4.681284	5.346772	7.339906	H	2.416902	10.336001	8.221971
C	8.293996	4.468949	7.056291	H	6.961217	16.716373	9.762229
C	5.849478	4.697522	7.206845	H	17.232583	6.880230	5.476399
C	13.013257	4.368941	6.090964	H	9.651141	7.397696	13.249559
C	14.400211	6.112652	6.712658	H	10.291617	7.385267	11.804690
C	14.171620	4.901363	6.195845	H	13.723465	6.605761	13.855622
C	15.696576	6.663996	6.703897	H	14.166707	6.605761	12.124663
C	15.912509	7.817145	7.614023	H	14.241429	8.118807	13.066026
C	2.972779	13.679083	10.034849	H	6.588593	4.580870	11.733615
C	4.364015	15.624718	10.797132	H	6.848845	4.580870	13.501369
C	3.169616	14.990115	10.656302	H	5.654966	5.688475	12.774100
PGc-DMM-enol							
C	11.220520	11.106847	9.806996	C	7.786129	11.298357	8.306057
C	11.405438	12.492488	10.206182	C	6.827892	13.475462	8.728023
C	12.700260	13.049933	10.524607	C	6.766054	12.221969	8.118046
C	13.886298	12.292110	10.477513	C	15.167503	5.888760	11.491193
C	12.315006	10.191482	9.764265	C	15.685997	7.148943	11.869125
C	15.049196	9.988397	9.546472	C	17.045200	7.362887	11.696826
C	12.264761	8.947999	9.133735	C	19.000950	8.708644	11.833072
C	15.176631	12.838861	10.482588	C	13.287550	4.436215	11.351263
C	16.258055	10.689997	9.507467	O	13.841803	5.731479	11.664360
C	16.355049	12.069403	10.089636	O	18.957214	14.482615	11.016564
C	9.804180	9.218122	9.186834	O	5.326378	9.985916	10.947324
C	9.954236	10.642302	9.381179	O	13.861944	10.017385	12.034427
C	17.369884	10.007112	8.868504	O	20.122698	11.820431	10.562819
C	17.197517	8.673751	8.358973	O	19.598631	13.158540	8.373430
C	12.830512	14.451721	10.831622	O	7.587314	9.201766	10.066023
C	15.284206	14.230848	10.844320	O	6.078696	7.469495	10.985525
C	14.115440	14.980387	11.042008	O	5.475047	8.522375	8.799818
C	10.291101	13.365604	10.164564	O	15.783485	3.029969	9.142862
C	9.047116	12.929363	9.603006	O	15.400749	2.325908	6.720769

C	8.902428	11.596970	9.115635	O	10.379593	3.255702	6.952793
C	17.575253	12.749894	10.189581	O	8.206691	4.540850	8.118377
C	16.565111	14.804514	11.048050	O	21.546640	6.033851	5.915034
C	17.674498	14.050229	10.778286	O	15.885674	4.940770	11.016123
C	18.659634	10.591014	8.745007	O	17.870630	6.447276	11.215444
C	19.703657	9.954926	8.100665	O	17.575073	8.543072	12.015783
C	19.558754	8.657160	7.590746	P	6.028267	8.893810	10.264744
C	18.303646	7.997453	7.756016	P	13.786573	10.555194	10.640781
C	18.188896	6.641613	7.327519	P	19.075525	12.198554	9.377476
C	14.796462	8.718177	8.927272	P	15.589138	3.485533	7.621914
C	13.471903	8.180606	8.818061	H	20.449461	12.646021	10.975214
C	10.956941	8.413301	8.890287	H	5.252312	7.264821	11.461104
C	10.815602	7.061684	8.494054	H	4.988784	9.279850	8.423396
C	12.001094	6.283741	8.170345	H	15.766631	3.751265	9.840837
C	15.924435	7.994798	8.412405	H	18.959557	15.437101	11.211967
C	15.789966	6.642164	7.995809	H	20.100893	4.147627	5.908293
C	16.967812	5.922297	7.522030	H	18.014172	2.850383	6.400579
C	14.472029	6.052196	7.998596	H	12.853933	3.131903	7.166858
C	13.315176	6.853114	8.314643	H	7.480953	6.674881	9.090716
C	11.670799	15.255556	10.904361	H	6.009689	14.189234	8.610332
C	10.424906	14.750783	10.567575	H	7.242561	15.857752	9.912994
C	9.526734	6.489599	8.488557	H	9.377649	16.630980	10.895977
C	8.427834	7.204914	8.986703	H	14.209242	16.029181	11.336345
C	8.574344	8.521284	9.374607	H	16.650902	15.829180	11.420223
C	16.976730	4.538480	7.221542	H	20.665344	10.464795	8.000566
C	14.256463	4.681365	7.660990	H	21.586067	8.562316	6.822455
C	11.855127	4.962571	7.709581	H	5.913655	11.969099	7.483773
C	9.300392	5.097548	8.055715	H	7.736160	10.333044	7.801478
C	12.986754	4.172025	7.474441	H	11.769661	16.311069	11.171699
C	10.527054	4.339403	7.509450	H	22.322403	6.617983	5.829937
C	18.086742	3.912644	6.643126	H	15.042442	7.942827	12.244894
C	19.315332	5.981476	6.735241	H	17.249430	5.632158	11.035406
C	19.240334	4.626840	6.373722	H	19.552177	8.054052	12.522429
C	20.534647	6.715390	6.528957	H	19.290028	8.482074	10.798512
C	20.650801	8.010684	6.953119	H	19.196543	9.762100	12.054486
C	7.969536	13.857539	9.444929	H	13.354733	4.231063	10.274174
C	9.271643	15.608892	10.525467	H	13.808866	3.643581	11.905585
C	8.100111	15.184578	9.983426	H	12.238008	4.493994	11.658648

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C	9.641975	10.790727	10.119772	C	7.444416	16.919085	10.073684
C	11.061457	10.800160	10.153406	C	6.794943	10.771938	10.054039
C	11.763350	12.037333	10.184744	C	21.707359	14.580705	10.048144
C	11.040417	13.268920	10.171055	C	10.986011	18.215170	10.124533
C	9.618408	13.257033	10.132994	C	18.099289	20.718616	10.053278
C	8.919239	12.021425	10.111011	C	15.977705	21.934551	10.056993
C	13.183485	12.047312	10.212129	C	5.337400	13.218542	10.032123
C	11.740236	14.505076	10.184836	C	5.307680	15.663461	10.033011
C	13.160612	14.516184	10.212481	C	11.066032	5.862992	10.086452
C	13.883626	13.284383	10.224255	C	8.944142	7.079331	10.063918
C	15.304744	13.294841	10.209184	C	9.702393	5.857337	10.063305
C	16.004124	14.531293	10.190061	C	4.638754	14.475189	10.019027
C	15.280552	15.761631	10.186254	C	5.364290	10.764360	10.023021
C	13.861016	15.751779	10.196964	C	4.671151	11.993221	10.013651

C	11.785507	9.567465	10.149943	C	6.813342	8.297917	10.034381
C	13.907925	10.813552	10.193053	C	7.549398	7.094117	10.036824
C	16.029743	12.061052	10.187008	C	5.387034	8.322559	10.005931
C	15.328027	10.826211	10.183246	C	4.691201	9.506741	10.001004
C	13.204393	9.578533	10.167188	C	17.341290	21.940569	10.042340
C	17.426090	14.542173	10.153407	C	21.679508	17.034527	10.033802
C	15.982465	16.997639	10.150831	C	22.373264	15.806077	10.027395
C	13.136706	16.984118	10.167945	C	20.230104	19.500584	10.037106
C	11.015264	15.738015	10.156775	C	22.352446	18.292133	10.010007
C	8.894279	14.489301	10.114424	C	21.656515	19.476250	10.011757
C	9.594462	15.723363	10.125878	C	19.494108	20.704254	10.032825
C	7.495284	12.010255	10.076618	C	11.795699	13.435815	5.132495
C	7.471042	14.472873	10.080970	C	13.050747	12.647103	5.398954
C	13.840013	18.218552	10.142848	C	13.618937	12.771362	6.815893
C	15.258610	18.229919	10.134466	C	14.546474	13.991695	6.845610
C	18.125162	15.777515	10.123543	C	16.004677	13.720650	6.590282
C	17.451178	12.075311	10.154467	O	13.620308	11.975334	4.547454
C	18.150970	13.309971	10.138631	O	14.093497	15.117552	7.020174
C	6.774320	13.239880	10.064133	H	15.891282	7.426503	10.132729
C	11.717167	16.971771	10.153258	H	20.156948	9.937862	10.089007
C	17.401783	17.007538	10.124001	H	18.024281	8.680801	10.121164
C	11.078708	8.332018	10.119525	H	22.289322	11.192168	10.043232
C	8.939204	9.552295	10.091310	H	9.020753	19.117226	10.083960
C	19.574333	13.326098	10.102453	H	11.153702	20.371302	10.092820
C	19.549004	15.788566	10.089695	H	13.288200	21.622702	10.078166
C	20.270460	14.559267	10.081068	H	6.888848	17.861095	10.057759
C	18.104422	18.245892	10.091639	H	13.755915	6.174656	10.118688
C	15.964970	19.465408	10.102495	H	23.498806	13.341401	10.011451
C	7.516591	9.543569	10.060455	H	9.155619	4.911276	10.042030
C	19.526976	18.254887	10.065024	H	3.546293	14.457877	9.995818
C	20.248989	17.026745	10.063562	H	3.577652	11.982147	9.989510
C	15.230396	20.705235	10.085706	H	7.007247	6.144252	10.015830
C	9.662359	8.323968	10.092752	H	4.850330	7.370771	9.987295
C	16.059280	9.582294	10.158288	H	17.887821	22.886791	10.019423
C	13.935553	8.335781	10.149965	H	15.422031	22.875534	10.045507
C	11.813652	7.092330	10.113156	H	23.466812	15.817934	10.003568
C	18.181488	10.832005	10.132648	H	4.756479	16.607014	10.020758
C	15.337944	8.369439	10.148761	H	11.621622	4.921881	10.084377
C	19.601164	10.879623	10.102280	H	3.598601	9.500943	9.979186
C	20.300007	12.081017	10.087105	H	22.193283	20.427937	9.992257
C	17.469835	9.623167	10.138515	H	23.445023	18.297802	9.988728
C	13.203396	7.118422	10.128116	H	20.036293	21.654003	10.009811
C	21.737755	12.135609	10.054272	H	11.548173	13.423851	4.065002
C	22.406231	13.324118	10.036594	H	10.964605	13.002309	5.712999
C	13.109380	19.461372	10.117898	H	11.923523	14.467910	5.497786
C	8.864057	16.966251	10.101766	H	16.110559	13.158417	5.647677
C	6.745365	15.717836	10.063168	H	16.569706	14.658630	6.548576
C	9.575527	18.175091	10.103903	H	16.408794	13.074225	7.385783
C	11.706928	19.428173	10.112869	H	14.168327	11.852365	7.056540
C	13.840776	20.679075	10.094110	H	12.809632	12.944272	7.536611
C	17.381285	19.474098	10.084075				
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C	9.672896	10.781383	10.046149	C	7.504933	16.917770	9.923695
C	11.092208	10.784935	10.093466	C	6.826418	10.774866	9.956508
C	11.799324	12.019043	10.124035	C	21.757105	14.516552	10.141542
C	11.082323	13.252691	10.095466	C	11.052062	18.196939	9.992984
C	9.661180	13.247078	10.043223	C	18.176798	20.669569	10.011438
C	8.955992	12.015125	10.023549	C	16.060558	21.894247	9.965254
C	13.219325	12.022505	10.161323	C	5.380078	13.227471	9.905674
C	11.787505	14.484659	10.105000	C	5.361968	15.672258	9.883207
C	13.207366	14.489481	10.148837	C	11.075073	5.847320	10.031034
C	13.925106	13.255432	10.178790	C	8.958756	7.072977	9.996267
C	15.345703	13.259305	10.195531	C	9.711537	5.847713	10.001783
C	16.051033	14.491872	10.188700	C	4.687410	14.487167	9.876387
C	15.333370	15.725555	10.156810	C	5.396013	10.773417	9.914657
C	13.913733	15.721816	10.136638	C	4.708193	12.005116	9.891915
C	11.810565	9.548792	10.097261	C	6.833823	8.300746	9.949499
C	13.938581	10.785332	10.158232	C	7.564351	7.093703	9.961284
C	16.065435	12.023036	10.189734	C	5.407956	8.331416	9.911232
C	15.358649	10.791329	10.171153	C	4.717502	9.518631	9.895062
C	13.229580	9.553412	10.126733	C	17.424307	21.894474	9.973305
C	17.473894	14.496883	10.183201	C	21.741137	16.970148	10.095843
C	16.041506	16.958292	10.120925	C	22.429150	15.738600	10.116055
C	13.195709	16.957224	10.082451	C	20.302383	19.442432	10.043515
C	11.069141	15.720009	10.055877	C	22.419678	18.224669	10.063298
C	8.942616	14.481805	10.005581	C	21.728901	19.411602	10.038327
C	9.648685	15.712221	10.010054	C	19.571739	20.649141	10.012383
C	7.532327	12.009943	9.976593	C	12.611726	11.247283	6.671137
C	7.519538	14.472003	9.959600	C	13.215553	12.623855	6.736393
C	13.905064	18.188314	10.056608	C	14.632814	12.795266	6.694582
C	15.323618	18.193562	10.074616	C	15.168988	14.074471	6.706042
C	18.179367	15.728890	10.152194	C	16.630140	14.370897	6.636252
C	17.487032	12.030581	10.186610	O	12.436934	13.631759	6.804924
C	18.193155	13.261682	10.184901	O	14.378520	15.132997	6.768030
C	6.816826	13.242354	9.948545	H	15.906910	7.388727	10.124620
C	11.776612	16.950680	10.046419	H	20.183756	9.880639	10.172009
C	17.461580	16.962145	10.121728	H	18.045780	8.632971	10.155253
C	11.098442	8.316511	10.062027	H	22.322929	11.125653	10.169927
C	8.964652	9.546026	10.016494	H	9.092321	19.108067	9.916411
C	19.617067	13.271709	10.172345	H	11.229797	20.351585	9.936687
C	19.603958	15.733930	10.138728	H	13.369653	21.593740	9.943243
C	20.319715	14.501450	10.153525	H	6.954575	17.862381	9.891094
C	18.170547	18.197006	10.083412	H	13.765944	6.146755	10.084176
C	16.036316	19.425550	10.040608	H	23.542925	13.269015	10.145686
C	7.542355	9.543366	9.974772	H	9.160559	4.904047	9.979945
C	19.593531	18.199848	10.079053	H	3.595006	14.474955	9.846117
C	20.310106	16.968660	10.105619	H	3.614751	11.998528	9.859763
C	15.307615	20.668385	9.995711	H	7.018154	6.146124	9.940077
C	9.682210	8.314513	10.026461	H	4.867252	7.381883	9.893679
C	16.084375	9.543828	10.157328	H	17.975607	22.837830	9.948565
C	13.955273	8.307212	10.116683	H	15.508870	22.837091	9.933477
C	11.827946	7.073394	10.061196	H	23.522993	15.744594	10.108041
C	18.211964	10.783745	10.176687	H	4.815363	16.618223	9.858128
C	15.357762	8.334286	10.133349	H	11.626497	4.903795	10.032037
C	19.632267	10.825177	10.175283	H	3.625032	9.517500	9.864764
C	20.337132	12.023349	10.173009	H	22.269844	20.360828	10.012048
C	17.495188	9.577790	10.164288	H	23.512543	18.225603	10.057293

C	13.217667	7.093202	10.087176	H	20.118383	21.596304	9.985490
C	21.775545	12.071550	10.165996	H	15.292548	11.930200	6.665157
C	22.450090	13.256798	10.152298	H	13.395929	14.709605	6.797417
C	13.180630	19.433847	10.004803	H	17.232977	13.469858	6.802711
C	8.924641	16.957983	9.963276	H	16.874975	14.786820	5.645791
C	6.799752	15.720014	9.922624	H	16.895241	15.133230	7.382409
C	9.641850	18.163486	9.955954	H	11.628440	11.247249	7.157516
C	11.778509	19.406540	9.976995	H	12.469051	10.967228	5.614523
C	13.917873	20.648018	9.979815	H	13.261259	10.492490	7.135056
C	17.452961	19.428175	10.046814				

G-CF<sub>3</sub>\_DK-Keto

C	9.699382	10.782447	9.971450	C	7.504990	16.908258	9.768831
C	11.118926	10.790442	9.961640	C	6.852330	10.766138	9.999471
C	11.821447	12.025396	9.895474	C	21.766947	14.570283	10.055619
C	11.099129	13.256086	9.837158	C	11.047794	18.200758	9.735178
C	9.676727	13.245890	9.856817	C	18.159466	20.706829	9.878191
C	8.977114	12.012123	9.921121	C	16.037924	21.921911	9.813771
C	13.242604	12.034422	9.906403	C	5.395384	13.211725	9.912626
C	11.799497	14.491388	9.788444	C	5.366428	15.655252	9.824251
C	13.221026	14.501951	9.801409	C	11.120310	5.859244	10.201660
C	13.944487	13.270442	9.860571	C	8.999378	7.075808	10.151553
C	15.365673	13.281061	9.896379	C	9.756652	5.854486	10.204484
C	16.065228	14.517524	9.878147	C	4.697169	14.468073	9.872452
C	15.341888	15.747900	9.828692	C	5.421540	10.759708	10.013218
C	13.922029	15.738307	9.789056	C	4.728571	11.987880	9.968795
C	11.842413	9.559286	10.025018	C	6.869353	8.294689	10.109157
C	13.966809	10.801928	9.976963	C	7.604539	7.091517	10.158722
C	16.089437	12.048414	9.961216	C	5.442871	8.320244	10.118534
C	15.386735	10.814785	9.997294	C	4.747622	9.503884	10.072837
C	13.261483	9.569165	10.030330	C	17.401169	21.928406	9.850619
C	17.486881	14.529421	9.924953	C	21.739553	17.024181	10.020166
C	16.043625	16.984770	9.838100	C	22.432949	15.795945	10.057528
C	13.197192	16.970783	9.762563	C	20.290075	19.489738	9.950282
C	11.075739	15.724669	9.763878	C	22.411940	18.282354	10.027411
C	8.953341	14.478263	9.821836	C	21.716040	19.466070	9.994267
C	9.654693	15.710936	9.777168	C	19.553837	20.692989	9.919271
C	7.553115	12.002576	9.938389	C	14.504244	15.172955	13.389380
C	7.529622	14.463412	9.841393	C	13.016783	15.211720	13.176491
C	13.900757	18.204994	9.772223	C	12.287709	13.869809	13.102109
C	15.319120	18.216732	9.808596	C	12.216007	13.103037	14.396404
C	18.185881	15.765240	9.924442	C	11.292976	11.838457	14.324991
C	17.510355	12.063505	9.995141	O	12.381971	16.250593	13.051391
C	18.210531	13.297699	9.977595	O	12.797747	13.360435	15.431432
C	6.832564	13.231716	9.895800	H	15.946874	7.418046	10.150862
C	11.778290	16.957701	9.747716	H	20.214830	9.928107	10.122976
C	17.462820	16.994938	9.884445	H	18.082167	8.671129	10.127617
C	11.134702	8.325838	10.086143	H	22.346920	11.182189	10.136459
C	8.995937	9.546109	10.036662	H	9.083682	19.104496	9.723829
C	19.633583	13.314940	10.018040	H	11.214584	20.356495	9.725412
C	19.609434	15.777120	9.969889	H	13.348337	21.608929	9.752459
C	20.330256	14.548193	10.012986	H	6.950514	17.850758	9.750252
C	18.165234	18.233780	9.895067	H	13.809900	6.168571	10.192939
C	16.025682	19.452694	9.823318	H	23.557302	13.331185	10.126628

C	7.573368	9.538534	10.047870	H	9.209444	4.909489	10.248724
C	19.587456	18.243446	9.939471	H	3.604442	14.451268	9.883673
C	20.309351	17.015652	9.975230	H	3.634789	11.977493	9.980968
C	15.290872	20.692291	9.799238	H	7.061940	6.142850	10.205848
C	9.718306	8.318695	10.090453	H	4.905623	7.369655	10.163910
C	16.117117	9.571704	10.061177	H	17.947437	22.874979	9.861471
C	13.991806	8.327521	10.093907	H	15.482279	22.862761	9.794713
C	11.868742	7.086979	10.144970	H	23.526249	15.808268	10.091606
C	18.239719	10.821040	10.053106	H	4.815254	16.598438	9.796625
C	15.394358	8.360479	10.103915	H	11.674857	4.918530	10.243616
C	19.659246	10.869231	10.082852	H	3.654881	9.498963	10.082211
C	20.358469	12.070426	10.067395	H	22.252422	20.418171	10.001862
C	17.527681	9.612638	10.082253	H	23.504274	18.288641	10.061335
C	13.258518	7.111953	10.146807	H	20.095558	21.643221	9.929220
C	21.796009	12.125488	10.102957	H	14.923942	16.183046	13.324693
C	22.464996	13.313813	10.097409	H	14.709834	14.738838	14.381459
C	13.170248	19.447580	9.754821	H	14.983013	14.516531	12.645192
C	8.924932	16.953922	9.756970	H	12.785559	13.206347	12.370398
C	6.804466	15.708373	9.808953	H	11.265755	14.031631	12.725911
C	9.637493	18.161730	9.733545	F	11.790080	10.964662	13.395983
C	11.768311	19.413630	9.733850	F	10.029778	12.180993	13.933282
C	13.901406	20.665512	9.766287	F	11.210656	11.198916	15.505870
C	17.441751	19.461683	9.864197				

G-CF<sub>3</sub>\_DK-enol

C	9.624802	10.774407	10.146035	C	7.464007	16.915470	10.095064
C	11.044427	10.776035	10.165320	C	6.777209	10.772568	10.070462
C	11.753472	12.007866	10.204101	C	21.712101	14.492912	10.057202
C	11.037469	13.243118	10.220187	C	11.012859	18.190960	10.150885
C	9.615139	13.240104	10.195441	C	18.140507	20.652252	10.069554
C	8.908618	12.008867	10.158891	C	16.026005	21.880579	10.064616
C	13.173331	12.009805	10.199389	C	5.334474	13.227801	10.044161
C	11.744349	14.475293	10.229134	C	5.320080	15.672837	10.038856
C	13.165275	14.477524	10.230955	C	11.019815	5.840506	10.016994
C	13.881595	13.241663	10.215818	C	8.905290	7.068541	10.032122
C	15.302290	13.244294	10.195320	C	9.656201	5.842367	10.007032
C	16.009230	14.475992	10.195520	C	4.643948	14.488712	10.020217
C	15.293684	15.710898	10.208914	C	5.346835	10.773668	10.026630
C	13.873387	15.709693	10.221722	C	4.661083	12.006614	10.015950
C	11.760865	9.539781	10.130665	C	6.781522	8.299063	10.023787
C	13.890554	10.772664	10.160076	C	7.510551	7.091199	10.010707
C	16.019590	12.007057	10.160658	C	5.355418	8.332264	9.989755
C	15.310398	10.777146	10.143532	C	4.666493	9.520415	9.990400
C	13.179414	9.542677	10.129358	C	17.389605	21.878532	10.050558
C	17.431026	14.479044	10.161881	C	21.698950	16.946955	10.054125
C	16.002413	16.943312	10.180430	C	22.385456	15.714390	10.042572
C	13.156033	16.947409	10.201430	C	20.263908	19.421509	10.057419
C	11.027193	15.712834	10.204875	C	22.379118	18.200710	10.029729
C	8.898124	14.476766	10.171767	C	21.689999	19.388823	10.030817
C	9.605820	15.706926	10.175039	C	19.535089	20.629633	10.048920
C	7.484749	12.006391	10.111587	C	9.683662	13.268528	6.743525
C	7.474957	14.469060	10.120905	C	11.181959	13.301031	6.740649
C	13.866924	18.177509	10.172227	C	11.889137	14.545912	6.671626
C	15.285741	18.179930	10.163581	C	13.263961	14.493742	6.586499

C	18.137434	15.710279	10.144402	C	14.112005	15.750379	6.408646
C	17.440685	12.012756	10.133780	O	11.828306	12.201151	6.763118
C	18.148060	13.242847	10.134958	O	13.939719	13.372867	6.597326
C	6.771024	13.240345	10.095175	H	15.852692	7.375288	10.045958
C	11.736304	16.943085	10.189740	H	20.133490	9.859003	10.042487
C	17.421747	16.944717	10.151363	H	17.993349	8.615477	10.051190
C	11.046926	8.308957	10.089554	H	22.273729	11.101376	10.019737
C	8.914661	9.540803	10.098623	H	9.053325	19.104074	10.094460
C	19.571375	13.250638	10.101007	H	11.193158	20.345198	10.102693
C	19.561214	15.713217	10.109298	H	13.334822	21.584129	10.086521
C	20.275223	14.479756	10.091364	H	6.914670	17.860807	10.065921
C	18.131453	18.178976	10.118124	H	13.710622	6.136696	10.025897
C	15.999376	19.411324	10.126082	H	23.496183	13.243210	10.010427
C	7.491985	9.540263	10.067279	H	9.104197	4.899659	9.975997
C	19.553864	18.179762	10.089243	H	3.551779	14.478567	9.982759
C	20.268505	16.947363	10.086492	H	3.567950	12.002113	9.979652
C	15.271946	20.655460	10.101586	H	6.963070	6.144700	9.977216
C	9.630627	8.308580	10.075942	H	4.813187	7.383908	9.959633
C	16.034004	9.529625	10.102029	H	17.941988	22.821108	10.020569
C	13.902814	8.296332	10.088561	H	15.475525	22.824404	10.045416
C	11.774187	7.065265	10.055239	H	23.479013	15.719558	10.016761
C	18.163591	10.765475	10.096214	H	4.775151	16.619869	10.014951
C	15.305343	8.321432	10.078270	H	11.570212	4.896699	9.993320
C	19.583612	10.804153	10.069223	H	3.574063	9.521318	9.960792
C	20.289810	12.001438	10.071433	H	22.231998	20.337542	10.008443
C	17.444733	9.560891	10.082708	H	23.471746	18.200203	10.007222
C	13.163931	7.083428	10.055819	H	20.082592	21.576305	10.021038
C	21.727831	12.047911	10.040775	H	9.326026	12.339523	7.203648
C	22.403561	13.232388	10.035074	H	11.364261	15.497217	6.681240
C	13.143508	19.424318	10.139437	H	9.261037	14.137804	7.264999
C	8.883598	16.954514	10.134031	H	9.327466	13.296988	5.700363
C	6.757558	15.718566	10.086528	H	13.127253	12.624762	6.683276
C	9.602347	18.158901	10.126484	F	13.459603	16.860811	6.853592
C	11.740999	19.399229	10.131224	F	15.290299	15.659176	7.070715
C	13.882092	20.637457	10.108849	F	14.396877	15.948833	5.086768
C	17.415649	19.411581	10.107204				

G-MAA-keto

C	9.647191	10.770162	10.051548	C	7.476909	16.905399	9.896143
C	11.066914	10.774045	10.090160	C	6.800581	10.762631	9.967502
C	11.773536	12.008799	10.113438	C	21.729971	14.514690	10.095884
C	11.055753	13.243119	10.088636	C	11.023074	18.185446	9.938966
C	9.633873	13.236506	10.045702	C	18.144062	20.664024	9.945425
C	8.929525	12.003814	10.030523	C	16.026932	21.886835	9.897627
C	13.194422	12.012944	10.144809	C	5.353463	13.214778	9.905803
C	11.760871	14.475592	10.079195	C	5.334402	15.659307	9.868100
C	13.181177	14.481329	10.109407	C	11.051132	5.836943	10.066902
C	13.899838	13.247559	10.148111	C	8.934441	7.061775	10.023268
C	15.321082	13.252237	10.163753	C	9.687628	5.836838	10.036689
C	16.025007	14.485230	10.132797	C	4.660289	14.473984	9.869269
C	15.306199	15.717722	10.090363	C	5.370202	10.760694	9.926004
C	13.886707	15.713449	10.078718	C	4.682157	11.992118	9.897951
C	11.786226	9.538348	10.100880	C	6.808732	8.288744	9.972103
C	13.914222	10.775661	10.153816	C	7.539803	7.082125	9.989887



C	16.041264	12.015532	10.179517	C	5.382786	8.318867	9.934107
C	15.334677	10.782825	10.173865	C	4.691992	9.505733	9.912178
C	13.205068	9.543548	10.132181	C	17.390533	21.888340	9.907755
C	17.447376	14.490995	10.124915	C	21.711441	16.968252	10.041306
C	16.013161	16.950815	10.049588	C	22.400675	15.737411	10.066089
C	13.167396	16.947708	10.022451	C	20.270456	19.438923	9.982495
C	11.041769	15.710278	10.021648	C	22.388908	18.223364	10.009927
C	8.915323	14.470822	9.997073	C	21.696962	19.409578	9.982328
C	9.621267	15.701271	9.984677	C	19.538925	20.645018	9.949735
C	7.505777	11.998029	9.983179	C	10.480819	13.162192	6.513826
C	7.492275	14.460227	9.951904	C	11.663274	12.737086	5.690558
C	13.875481	18.178762	9.988806	C	13.028923	12.681106	6.383057
C	15.294036	18.185089	10.003403	C	13.614880	14.061674	6.646616
C	18.151499	15.723604	10.086493	C	15.810524	12.987890	6.748677
C	17.463188	12.024093	10.172775	O	11.577868	12.412935	4.512698
C	18.167807	13.256133	10.147703	O	12.953772	15.080693	6.730169
C	6.790186	13.230196	9.948958	O	14.964553	14.152606	6.815400
C	11.748669	16.940300	9.995977	H	15.883067	7.380431	10.163448
C	17.432777	16.955759	10.051789	H	20.161734	9.876793	10.180828
C	11.074036	8.305920	10.077712	H	18.023100	8.626493	10.185946
C	8.939375	9.534589	10.029130	H	22.299969	11.124676	10.155313
C	19.591843	13.267442	10.135571	H	9.062837	19.095636	9.867925
C	19.575735	15.729738	10.079802	H	11.198202	20.339783	9.872009
C	20.292706	14.498029	10.104891	H	13.336451	21.583542	9.872489
C	18.140244	18.191242	10.015544	H	6.926502	17.849707	9.858564
C	16.005228	19.417864	9.969541	H	13.741577	6.137167	10.123672
C	7.516995	9.531576	9.990553	H	23.516966	13.268929	10.109677
C	19.562927	18.195621	10.015613	H	9.136898	4.893003	10.020700
C	20.280560	16.965223	10.046035	H	3.567923	14.460979	9.839703
C	15.275476	20.660145	9.925473	H	3.588685	11.985219	9.866421
C	9.657732	8.303625	10.044169	H	6.993684	6.134289	9.975490
C	16.061033	9.535574	10.174729	H	4.842168	7.369226	9.921115
C	13.931294	8.297829	10.138221	H	17.941042	22.832203	9.885271
C	11.803845	7.063236	10.088276	H	15.474358	22.829103	9.867015
C	18.188673	10.777388	10.178585	H	23.494583	15.744604	10.060577
C	15.333894	8.326016	10.160913	H	4.787662	16.604967	9.837431
C	19.609108	10.820636	10.172524	H	11.602510	4.893529	10.075809
C	20.312733	12.019646	10.152174	H	3.599512	9.504230	9.881922
C	17.472055	9.570928	10.182761	H	22.236942	20.359499	9.958484
C	13.193587	7.083633	10.117394	H	23.481750	18.225500	10.007769
C	21.751144	12.069645	10.142410	H	20.084446	21.592823	9.924573
C	22.424078	13.255655	10.116556	H	9.586880	13.238980	5.885083
C	13.150177	19.423607	9.936543	H	10.308106	12.423959	7.314197
C	8.896414	16.946177	9.929798	H	10.697762	14.122288	7.005993
C	6.772099	15.707601	9.905711	H	13.693464	12.077597	5.751389
C	9.612966	18.151543	9.910173	H	12.938713	12.177319	7.362627
C	11.748111	19.395443	9.913647	H	15.450166	12.182858	7.404605
C	13.885816	20.638538	9.909213	H	15.898234	12.625856	5.712982
C	17.421703	19.421740	9.977901	H	16.792076	13.322809	7.104131
G-MAA-enol							
C	9.630058	10.780956	10.074320	C	7.469457	16.921556	10.012800
C	11.049480	10.782616	10.088748	C	6.782306	10.778896	10.019162
C	11.758600	12.014878	10.118937	C	21.718750	14.498333	10.047595

C	11.043134	13.249958	10.132528	C	11.018016	18.196663	10.065527
C	9.621315	13.246960	10.107849	C	18.147306	20.658691	10.037600
C	8.914406	12.015571	10.080793	C	16.032543	21.886929	10.024381
C	13.178521	12.016285	10.120025	C	6.785797	8.305069	9.998569
C	11.749678	14.481611	10.144209	C	7.514542	7.096977	9.994553
C	13.170100	14.483490	10.151268	C	5.359487	8.338122	9.975449
C	13.886160	13.247876	10.139902	C	4.670826	9.526428	9.968847
C	15.306834	13.249685	10.129030	C	17.396296	21.884991	10.022387
C	16.014090	14.481311	10.132723	C	21.705929	16.952583	10.043731
C	15.298002	15.716740	10.137586	C	22.392296	15.719842	10.039759
C	13.877925	15.715506	10.142858	C	5.339694	13.233855	9.985265
C	11.765651	9.546043	10.066266	C	5.325188	15.678733	9.969470
C	13.895514	10.778831	10.091005	C	11.023699	5.845854	9.999732
C	16.024483	12.012470	10.100728	C	8.909368	7.074369	10.007778
C	15.315338	10.782598	10.083443	C	9.660031	5.847852	9.994842
C	13.184379	9.548618	10.066985	C	4.648954	14.494554	9.959778
C	17.436462	14.484523	10.107462	C	5.351685	10.779831	9.986911
C	16.007654	16.949188	10.111122	C	4.665997	12.012682	9.970917
C	13.161054	16.952946	10.117105	C	20.270945	19.427731	10.038831
C	11.032686	15.718680	10.118641	C	22.386215	18.206507	10.030310
C	8.904196	14.483203	10.084316	C	21.697239	19.394770	10.027824
C	9.611720	15.713028	10.087026	C	19.542120	20.635973	10.030334
C	7.490239	12.012900	10.043922	C	9.504702	13.413563	6.551310
C	7.480982	14.475343	10.041215	C	10.996111	13.403374	6.555525
C	13.871924	18.183268	10.091928	C	11.771534	14.533348	6.642594
C	15.290982	18.186136	10.091291	C	13.204778	14.413948	6.611934
C	18.143314	15.715883	10.093266	C	15.300454	15.524350	6.625623
C	17.445831	12.018042	10.084812	O	11.532290	12.182166	6.454355
C	18.153669	13.247972	10.088928	O	13.820708	13.325960	6.518835
C	6.776610	13.246714	10.025291	O	13.860054	15.598683	6.693575
C	11.741431	16.948797	10.103689	H	15.857498	7.379910	10.015226
C	17.427593	16.950573	10.093229	H	20.139147	9.864305	10.029718
C	11.051560	8.314925	10.040589	H	17.998541	8.620394	10.025336
C	8.919552	9.547054	10.044305	H	22.280102	11.106613	10.025938
C	19.577389	13.256061	10.069239	H	9.058617	19.110174	10.010809
C	19.567501	15.718891	10.072971	H	11.198388	20.351168	10.023037
C	20.281460	14.485155	10.064965	H	13.340749	21.590326	10.021875
C	18.137814	18.185013	10.070249	H	6.920139	17.866983	9.985957
C	16.005342	19.417652	10.065397	H	13.714772	6.141351	10.002501
C	7.496769	9.546456	10.022916	H	23.502893	13.248043	10.024379
C	19.560570	18.185764	10.056847	H	9.107600	4.905012	9.978902
C	20.275097	16.953129	10.059064	H	3.556515	14.484022	9.930099
C	15.277798	20.661873	10.044443	H	3.572494	12.007966	9.943450
C	9.635145	8.314632	10.032403	H	6.966709	6.150278	9.976515
C	16.038813	9.534665	10.055301	H	4.816908	7.389609	9.960413
C	13.907538	8.301655	10.041089	H	17.948868	22.827801	10.006685
C	11.778528	7.070778	10.020491	H	15.482272	22.830908	10.009788
C	18.168755	10.770452	10.059432	H	23.486107	15.724751	10.026853
C	15.310167	8.326377	10.036538	H	4.779925	16.625654	9.947273
C	19.589079	10.809484	10.046404	H	11.573711	4.901568	9.987334
C	20.295681	12.006621	10.051645	H	3.578176	9.527457	9.948228
C	17.449747	9.565937	10.046325	H	22.239632	20.343494	10.015720
C	13.168361	7.088624	10.020421	H	23.479063	18.206104	10.020010
C	21.733992	12.053122	10.037346	H	20.089830	21.582769	10.015180
C	22.410019	13.237531	10.036429	H	9.122254	12.699937	7.295585

C	13.148606	19.430387	10.061651	H	11.314780	15.514809	6.740452
C	8.889195	16.960287	10.047818	H	9.109609	14.412307	6.771296
C	6.763030	15.724601	10.008657	H	9.133589	13.086303	5.567375
C	9.607623	18.164961	10.040854	H	12.542302	12.332469	6.458925
C	11.746209	19.405159	10.049538	H	15.689263	14.791962	7.345180
C	13.887836	20.643511	10.041668	H	15.618605	15.237730	5.612793
C	17.421907	19.417822	10.059082	H	15.654007	16.531755	6.871511
G-DMM-keto							
C	9.552114	10.723683	10.275765	C	6.704877	10.734652	10.209402
C	10.972156	10.718783	10.298946	C	21.661613	14.371147	10.141064
C	11.687760	11.947803	10.281156	C	10.980447	18.125164	9.957213
C	10.978439	13.185301	10.237625	C	18.124651	20.541166	9.798228
C	9.556866	13.188964	10.206988	C	16.016804	21.778364	9.719091
C	8.842992	11.961428	10.229602	C	5.274722	13.194863	10.100071
C	13.108023	11.941667	10.288333	C	5.272740	15.638269	10.004286
C	11.692024	14.412081	10.195231	C	10.921531	5.781958	10.383912
C	13.112796	14.406625	10.205448	C	8.813335	7.020328	10.330307
C	13.822468	13.168368	10.255075	C	9.557974	5.790441	10.363883
C	15.242523	13.162612	10.254558	C	4.590336	14.457989	10.038445
C	15.956470	14.388949	10.205248	C	5.274280	10.741940	10.175830
C	15.248202	15.627069	10.145723	C	4.594646	11.977194	10.124413
C	13.827759	15.633379	10.143286	C	6.696050	8.261065	10.266520
C	11.682318	9.478498	10.329227	C	7.418745	7.049765	10.305273
C	13.818464	10.700894	10.319818	C	5.270072	8.300632	10.235216
C	15.953425	11.922574	10.289442	C	4.587544	9.491786	10.192270
C	15.238092	10.697285	10.322798	C	17.380512	21.768934	9.716070
C	13.101162	9.474406	10.341894	C	21.662762	16.821880	10.008854
C	17.378923	14.383936	10.191438	C	22.342056	15.586788	10.070758
C	15.964167	16.853460	10.067153	C	20.241577	19.300545	9.868300
C	13.117827	16.872749	10.060482	C	22.350269	18.069263	9.927470
C	10.981317	15.650919	10.115091	C	21.667797	19.259325	9.859377
C	8.846051	14.427297	10.134853	C	19.519302	20.510212	9.793474
C	9.559865	15.652233	10.087333	C	11.865488	13.984913	6.014520
C	7.418854	11.964946	10.192451	C	12.644588	15.185498	6.509054
C	7.422570	14.425985	10.101506	C	14.120049	14.853475	6.655461
C	13.835859	18.096558	9.978694	C	16.294333	15.794098	6.671998
C	15.254498	18.091238	9.981074	C	10.517423	12.155434	6.666069
C	18.092838	15.609625	10.121329	O	11.805920	13.632691	4.849098
C	17.374582	11.919939	10.282671	O	14.579162	13.743530	6.861259
C	18.089310	13.144213	10.233883	O	14.865011	15.982970	6.547003
C	6.711761	13.201180	10.133517	O	11.241581	13.351153	7.036400
C	11.697345	16.875891	10.047448	H	15.763033	7.292237	10.401547
C	17.384010	16.846598	10.056836	H	20.055603	9.751178	10.342901
C	10.961700	8.250867	10.341768	H	17.909567	8.520784	10.378983
C	8.835508	9.492952	10.285197	H	22.203747	10.979454	10.290351
C	19.513023	13.143650	10.219664	H	9.025960	19.046877	9.878776
C	19.517227	15.603540	10.102130	H	11.174196	20.274109	9.814429
C	20.224194	14.366952	10.156839	H	13.323889	21.498507	9.740632
C	18.101147	18.073788	9.967225	H	6.879481	17.816181	9.924709
C	15.975616	19.315514	9.892097	H	13.614415	6.064824	10.411669
C	7.412956	9.499151	10.255260	H	23.438833	13.111929	10.185865
C	19.523930	18.065781	9.954383	H	9.000881	4.850093	10.371473
C	20.231846	16.831314	10.023705	H	3.497612	14.452226	10.016143

C	15.255078	20.560631	9.805777	H	3.500953	11.977255	10.099322
C	9.545252	8.257209	10.320502	H	6.866269	6.105832	10.313777
C	15.954988	9.445833	10.354081	H	4.722765	7.354704	10.244363
C	13.817926	8.223764	10.371696	H	17.938122	22.706553	9.648998
C	11.682676	7.003231	10.372860	H	15.472077	22.723469	9.654190
C	18.090950	10.669394	10.318583	H	23.435926	15.585014	10.059149
C	15.220536	8.241356	10.379418	H	4.732188	16.586817	9.954676
C	19.511351	10.699445	10.312344	H	11.466626	4.835089	10.407802
C	20.224764	11.891329	10.264374	H	3.494952	9.497339	10.167679
C	17.365932	9.469217	10.354435	H	22.215305	20.202822	9.795092
C	13.072584	7.014556	10.388492	H	23.443039	18.061935	9.917857
C	21.663319	11.928630	10.252987	H	20.072342	21.451715	9.728024
C	22.346069	13.107681	10.195085	H	12.274143	15.516165	7.491295
C	13.118998	19.344391	9.888984	H	12.524683	16.010872	5.796284
C	8.844187	16.901114	10.004512	H	16.530029	15.188690	7.556077
C	6.711113	15.677265	10.029809	H	16.683746	15.291148	5.775758
C	9.569589	18.100220	9.943390	H	16.714302	16.800896	6.766413
C	11.716184	19.326832	9.882774	H	9.774044	12.382986	5.889953
C	13.865152	20.550514	9.806990	H	11.215140	11.395696	6.287951
C	17.392040	19.307743	9.886872	H	10.030868	11.812350	7.585234
C	7.423942	16.869423	9.983243				
G-DMM-enol							
C	9.589270	10.662603	10.218876	C	6.742515	10.615860	10.163609
C	11.008999	10.685852	10.232466	C	21.621656	14.554660	10.009115
C	11.700111	11.928694	10.217485	C	10.866658	18.091951	9.935694
C	10.965764	13.152461	10.184062	C	17.958195	20.656626	9.776395
C	9.543648	13.127511	10.162230	C	15.824899	21.851313	9.721422
C	8.855203	11.885998	10.182976	C	5.262479	13.046664	10.056529
C	13.119830	11.951200	10.217027	C	5.211646	15.489308	9.960419
C	11.653912	14.393993	10.147182	C	11.058064	5.747969	10.290807
C	13.074313	14.417484	10.154216	C	8.925172	6.944186	10.260330
C	13.809013	13.193171	10.188863	C	9.694366	5.729280	10.282186
C	15.229424	13.215973	10.174216	C	4.552852	14.295755	9.994304
C	15.917777	14.457155	10.128856	C	5.312160	10.594211	10.133084
C	15.183438	15.681068	10.091584	C	4.607535	11.815458	10.082184
C	13.763370	15.658730	10.100453	C	6.783289	8.142184	10.214820
C	11.743873	9.459838	10.250365	C	7.530145	6.945457	10.244494
C	13.855177	10.724896	10.231849	C	5.356674	8.153065	10.191045
C	15.965260	11.989704	10.190628	C	4.650512	9.330489	10.151706
C	15.274789	10.749588	10.220892	C	17.188641	21.869936	9.712228
C	13.162457	9.484122	10.250772	C	21.572392	17.006586	9.910386
C	17.339945	14.480700	10.100251	C	22.276836	15.784660	9.948385
C	15.874776	16.922434	10.020293	C	20.100582	19.458612	9.816699
C	13.028210	16.883238	10.029778	C	22.233858	18.268904	9.841799
C	10.918224	15.618306	10.077670	C	21.527370	19.446117	9.797117
C	8.808626	14.351184	10.094482	C	19.353374	20.654415	9.762229
C	9.497785	15.590523	10.051171	C	11.901736	13.782213	6.728603
C	7.431466	11.860453	10.147887	C	12.552637	15.043136	6.710341
C	7.385591	14.320878	10.059545	C	13.939063	15.026101	6.685652
C	13.720922	18.121750	9.955252	C	9.876937	12.548713	6.734600
C	15.139532	18.146135	9.951362	C	16.057821	16.101889	6.603941
C	18.028734	15.721096	10.038469	O	12.516381	12.670559	6.718535
C	17.386135	12.015839	10.169169	O	14.634497	13.908989	6.673715

C	18.075418	13.255168	10.123894	O	10.550405	13.824415	6.764294
C	6.699325	13.082119	10.089833	O	14.616851	16.180954	6.680543
C	11.608730	16.857338	10.017989	H	15.867530	7.354901	10.267839
C	17.294491	16.944321	9.996651	H	20.110657	9.901542	10.181561
C	11.048355	8.217680	10.261997	H	17.989981	8.626808	10.232788
C	8.897917	9.417381	10.226479	H	22.231716	11.172571	10.114025
C	19.498695	13.283537	10.095448	H	8.893733	18.974533	9.858074
C	19.452728	15.744062	10.006227	H	11.015756	20.245771	9.808243
C	20.184885	14.521408	10.039027	H	13.137967	21.514252	9.746283
C	17.986076	18.186930	9.915874	H	6.773644	17.699612	9.890268
C	15.834986	19.385771	9.869379	H	13.744838	6.085161	10.292224
C	7.475312	9.394754	10.203916	H	23.423508	13.329635	10.019108
C	19.408707	18.208181	9.891401	H	9.155742	4.778192	10.289970
C	20.141655	16.987103	9.937815	H	3.460709	14.268361	9.971759
C	15.088871	20.616940	9.798353	H	3.514131	11.793225	10.058213
C	9.632039	8.195755	10.251540	H	6.996245	5.990728	10.251467
C	16.016836	9.512319	10.234937	H	4.828396	7.196509	10.202800
C	13.904255	8.247903	10.264885	H	17.727137	22.819153	9.652943
C	11.794250	6.984483	10.279242	H	15.259638	22.785278	9.668752
C	18.127329	10.779121	10.187213	H	23.370268	15.805300	9.926240
C	15.306319	8.293398	10.258541	H	4.652322	16.426802	9.909374
C	19.546623	10.838533	10.165667	H	11.622211	4.812108	10.305503
C	20.235216	12.045110	10.120317	H	3.557997	9.314854	10.131361
C	17.426962	9.564171	10.221092	H	22.055862	20.401327	9.743463
C	13.183579	7.023735	10.281098	H	23.326336	18.283684	9.823552
C	21.672455	12.111267	10.092980	H	19.887104	21.607685	9.704153
C	22.331125	13.304239	10.040555	H	11.999043	15.975848	6.732567
C	12.978991	19.355452	9.876221	H	13.864287	13.154517	6.692389
C	8.756538	16.824772	9.972463	H	10.001930	12.073708	5.750647
C	6.648865	15.557495	9.988618	H	10.269326	11.878431	7.510478
C	9.456642	18.039026	9.919004	H	8.821778	12.776349	6.921452
C	11.577100	19.309372	9.870229	H	16.460154	15.473495	7.409155
C	13.699556	20.577610	9.803248	H	16.367266	15.694710	5.630750
C	17.251413	19.407139	9.855377	H	16.404171	17.134695	6.717914
C	7.337363	16.764126	9.947354				

GO-AA-keto (above)

C	19.055614	11.078332	10.326358	C	8.424192	14.971971	9.988726
C	18.392363	12.278502	10.456516	C	7.725267	13.770138	9.945037
C	19.129837	13.549826	10.419836	C	8.367701	12.534824	10.152199
C	20.521976	13.557441	10.229545	C	10.351655	6.382780	9.516690
C	21.286427	12.303997	10.247565	C	9.621052	7.598874	9.740587
C	20.519871	11.012321	10.274882	C	8.281748	10.083447	10.068138
C	18.435190	14.797949	10.486079	C	8.239257	7.644306	9.630193
C	21.244019	14.760961	10.030809	C	7.478471	8.856053	9.813481
C	20.565037	15.985435	10.158504	C	7.649111	11.314011	10.052631
C	19.173069	16.027514	10.378660	C	14.641150	6.276963	9.583469
C	21.355478	17.226782	10.158244	C	12.492456	5.160398	9.252175
C	22.711634	17.188103	9.590813	C	13.860357	5.142497	9.221286
C	23.355980	15.973018	9.475290	C	7.573481	16.176886	9.753048
C	22.667219	14.739016	9.761400	C	9.606872	5.129634	9.174249
C	23.352728	13.521304	9.655799	C	17.071424	17.258450	12.460109
C	22.659670	12.299980	9.714455	C	13.914592	12.029669	14.200357
C	16.950737	12.287199	10.590349	C	15.176173	12.246897	14.984114

C	16.267494	13.566402	10.962457	C	15.166655	13.466784	15.952395
C	17.011744	14.829584	10.596366	C	15.951597	14.619089	15.365187
C	16.300255	16.023403	10.571037	C	17.442076	14.534997	15.413550
C	17.038193	17.314833	10.846272	O	26.624624	12.997021	11.185988
C	18.490419	17.291800	10.434765	O	24.737968	14.040661	11.898970
C	20.616150	18.534925	10.180355	O	16.343431	13.576002	12.461591
C	19.143957	18.488981	10.224652	O	21.247501	18.016802	11.392042
C	24.734402	15.930652	9.000644	O	21.192041	22.053982	9.171045
C	25.424694	14.767334	8.981134	O	18.416216	5.791815	7.726944
C	21.294746	19.726143	9.612096	O	19.864576	5.778259	9.467331
C	23.359505	18.425747	9.200219	O	14.356122	7.799734	11.506543
C	22.608625	19.652622	9.227697	O	21.180784	11.513844	11.479460
C	18.434177	19.731174	10.090083	O	14.165929	19.620682	10.008082
C	17.035582	19.718477	10.144349	O	26.580957	17.181759	8.108789
C	16.300571	18.554337	10.390123	O	10.254996	11.186420	12.266993
C	14.875216	16.040504	10.557377	O	6.488332	16.144312	9.188912
C	14.143559	14.846559	10.652821	O	8.072255	17.348532	10.255230
C	14.793967	13.599315	10.659381	O	9.668390	4.548601	8.102240
C	16.202261	11.121989	10.486893	O	8.849631	4.680899	10.214109
C	16.860737	9.861625	10.285013	O	18.084867	17.014427	13.086897
C	18.349209	9.766615	10.492346	O	15.846332	17.383778	12.986225
C	21.137905	9.841411	9.627724	O	6.229427	8.876698	9.759625
C	22.470125	9.903470	9.224593	O	25.017950	9.956415	8.189651
C	23.233246	11.088909	9.282835	O	18.546804	9.353630	11.900849
C	18.986729	8.623940	9.718515	O	12.581818	14.964294	12.459921
C	20.329472	8.720544	9.365294	O	16.163071	11.532099	14.909891
C	24.595812	11.133506	8.752926	O	15.339745	15.565518	14.841165
C	25.347929	12.252846	8.810128	H	26.467386	14.772797	8.651276
C	25.422522	17.197449	8.568462	H	23.106903	20.557287	8.874916
C	24.662090	18.414482	8.727736	H	16.531076	20.659031	9.896176
C	20.512077	20.927137	9.534811	H	22.925997	9.017765	8.779496
C	19.157156	20.923098	9.788253	H	18.595106	21.858055	9.696264
C	14.904643	18.505081	10.269466	H	25.153013	19.343626	8.430780
C	14.159587	17.303398	10.392346	H	26.379219	12.260476	8.451818
C	14.063388	12.410480	10.594563	H	20.806108	7.878954	8.859597
C	14.743527	11.153796	10.508891	H	25.241987	14.030915	12.741680
C	24.855236	13.486155	9.517227	H	15.747581	14.301424	12.746712
C	25.522993	13.455264	10.965833	H	20.573490	22.805775	9.117334
C	18.196487	7.484773	9.438286	H	16.498468	5.414701	9.059792
C	16.161018	8.692553	10.105157	H	12.266576	18.233728	10.010662
C	14.005774	9.979933	10.407142	H	20.181915	5.008482	8.946002
C	12.614223	12.436791	10.579777	H	6.653703	13.795575	9.741300
C	12.670074	14.902934	10.965115	H	14.742582	20.406197	10.011954
C	12.775891	17.301231	10.257926	H	6.569145	11.328189	9.881250
C	16.807304	7.467422	9.694064	H	14.383581	4.241190	8.892017
C	14.711969	8.690963	10.389777	H	11.943184	4.266517	8.957357
C	12.568258	9.987988	10.384053	H	10.569441	10.306373	12.558010
C	11.897556	11.200182	10.513035	H	7.392078	18.024565	10.045752
C	11.923400	13.648742	10.636090	H	8.389889	3.873093	9.895402
C	12.003529	16.132153	10.412678	H	15.817693	16.888811	13.866958
C	10.644199	16.134199	10.152061	H	10.185488	17.077961	9.863461
C	13.923562	7.440871	10.149179	H	7.659784	6.746691	9.414021
C	16.009981	6.311374	9.442247	H	25.945105	10.053451	7.904076
C	18.807434	6.291744	8.771562	H	18.066584	9.992423	12.468565
C	10.498791	13.702810	10.444446	H	13.033262	15.787602	12.741312

C	10.418051	11.215543	10.783587	H	14.052849	11.225489	13.469085
C	11.816680	8.752849	10.159159	H	13.098474	11.765520	14.893817
C	12.463453	7.546826	9.940842	H	13.595456	12.958562	13.697956
C	11.743596	6.350105	9.567491	H	17.754597	13.534073	15.073151
C	10.377594	8.810641	10.055382	H	17.908369	15.321340	14.808733
C	9.695315	10.005196	10.246490	H	17.770435	14.619820	16.462986
C	9.759782	12.518167	10.414402	H	15.649229	13.124246	16.878929
C	9.836248	14.970481	10.221933	H	14.138750	13.798229	16.143446
GO-AA-enol (above)							
C	19.056486	11.284094	10.246878	C	8.392108	15.079352	9.949896
C	18.392864	12.475897	10.438154	C	7.697187	13.875350	9.955534
C	19.127535	13.751370	10.422398	C	8.353382	12.649531	10.174629
C	20.523201	13.764164	10.243162	C	10.375944	6.509512	9.580205
C	21.289139	12.509928	10.231467	C	9.639992	7.721539	9.810727
C	20.520010	11.219271	10.186616	C	8.286441	10.198110	10.126138
C	18.422527	14.996362	10.470108	C	8.256466	7.755063	9.718771
C	21.244978	14.971139	10.051770	C	7.489651	8.965164	9.879284
C	20.553665	16.192425	10.139975	C	7.643301	11.422948	10.104853
C	19.153896	16.227720	10.324686	C	14.664081	6.480318	9.429565
C	21.330639	17.442911	10.119815	C	12.522496	5.324981	9.205385
C	22.710943	17.404629	9.613329	C	13.886095	5.336269	9.093514
C	23.367434	16.192741	9.540133	C	7.533334	16.279881	9.726258
C	22.675386	14.956711	9.812220	C	9.633946	5.238450	9.307517
C	23.366552	13.741725	9.707706	C	16.973108	17.731892	12.217259
C	22.671234	12.520887	9.719500	C	15.333685	9.640411	14.098574
C	16.949631	12.478727	10.591003	C	16.411919	10.665446	14.297005
C	16.266272	13.758341	10.991987	C	17.770136	10.253879	14.470848
C	16.997864	15.022897	10.580645	C	18.788363	11.188978	14.636970
C	16.271578	16.200500	10.494791	C	20.231106	10.838931	14.730297
C	16.986864	17.529280	10.632176	O	26.617216	13.175096	11.270814
C	18.457840	17.482744	10.278847	O	24.729383	14.217064	11.985415
C	20.572975	18.744646	10.045133	O	16.380106	13.888056	12.457747
C	19.103384	18.674507	10.010456	O	21.150545	18.287310	11.304564
C	24.762016	16.156521	9.112078	O	21.160625	22.228918	8.928144
C	25.454163	14.995329	9.097141	O	18.361755	6.176945	7.320538
C	21.266169	19.922052	9.466745	O	19.847427	6.047504	9.025337
C	23.365398	18.640192	9.222850	O	14.431473	7.932826	11.419027
C	22.602465	19.857145	9.170369	O	21.172686	11.657695	11.423507
C	18.382938	19.885836	9.730418	O	14.131282	19.662218	9.380580
C	16.985453	19.839127	9.668618	O	26.647457	17.411242	8.312887
C	16.256775	18.689087	9.982018	O	10.259237	11.351033	12.290096
C	14.844014	16.202383	10.453161	O	6.435837	16.243271	9.186886
C	14.121148	15.015002	10.625062	O	8.043462	17.449379	10.220827
C	14.783877	13.775051	10.695999	O	9.686563	4.596734	8.269581
C	16.208933	11.307465	10.469278	O	8.887578	4.843819	10.377940
C	16.869822	10.059161	10.203752	O	17.906040	17.471325	12.945232
C	18.365250	9.957945	10.341974	O	15.768966	18.178919	12.648409
C	21.136448	10.083446	9.478369	O	6.241186	8.982996	9.806226
C	22.478043	10.152420	9.111195	O	25.057327	10.215512	8.171977
C	23.248585	11.324883	9.250664	O	18.636616	9.421603	11.692204
C	18.979742	8.879278	9.465023	O	12.471942	15.373267	12.324047
C	20.322428	8.993284	9.121185	O	16.100483	11.902496	14.306308
C	24.624020	11.378362	8.756989	O	18.525492	12.482708	14.671960



C	25.377865	12.491647	8.865799	H	26.505888	15.006995	8.797068
C	25.465754	17.424356	8.709632	H	23.108734	20.755733	8.813812
C	24.689178	18.634958	8.813540	H	16.483227	20.743172	9.305662
C	20.472485	21.102461	9.278995	H	22.934986	9.289489	8.624512
C	19.101933	21.076626	9.415400	H	18.529127	21.989891	9.224557
C	14.868488	18.603846	9.820440	H	25.182899	19.564377	8.522521
C	14.128129	17.427505	10.108198	H	26.418106	12.506270	8.535077
C	14.060203	12.578094	10.623449	H	20.799164	8.185165	8.563711
C	14.747868	11.326015	10.513182	H	25.228989	14.194744	12.830526
C	24.871759	13.706260	9.595663	H	16.019028	13.076313	12.891657
C	25.519815	13.643120	11.048782	H	20.534464	22.963087	8.788758
C	18.185383	7.755992	9.142158	H	16.502962	5.675293	8.765918
C	16.172176	8.896634	9.978458	H	12.245737	18.293795	9.565769
C	14.017621	10.148191	10.391638	H	20.151470	5.312970	8.448078
C	12.609036	12.592134	10.590543	H	6.620210	13.890737	9.780212
C	12.634665	15.080160	10.871786	H	14.710568	20.434757	9.249965
C	12.749244	17.402006	9.941399	H	6.561465	11.425756	9.945565
C	16.811735	7.706626	9.466463	H	14.406242	4.450971	8.719005
C	14.734103	8.866481	10.312552	H	11.974707	4.423967	8.931732
C	12.578867	10.142647	10.390844	H	10.568255	10.474310	12.596444
C	11.900581	11.348248	10.536018	H	7.359629	18.127495	10.030718
C	11.908702	13.800983	10.597633	H	8.427710	4.019266	10.106107
C	11.976117	16.260468	10.212551	H	15.800817	18.170372	13.628907
C	10.614975	16.242470	9.967616	H	10.152652	17.159554	9.605905
C	13.955788	7.616638	10.061416	H	7.681264	6.851343	9.517947
C	16.020615	6.548022	9.208066	H	25.991894	10.318157	7.913747
C	18.776865	6.607725	8.386019	H	18.223898	10.015371	12.360821
C	10.480941	13.834731	10.407729	H	12.911139	14.645364	12.809500
C	10.420239	11.356097	10.806876	H	18.018297	9.193749	14.476410
C	11.834572	8.901780	10.166048	H	17.500044	12.552881	14.549454
C	12.487341	7.705611	9.913301	H	20.379391	9.759644	14.848695
C	11.769680	6.499329	9.566505	H	20.731842	11.165762	13.803343
C	10.392412	8.943372	10.098023	H	20.696848	11.380902	15.565966
C	9.702679	10.133204	10.290809	H	14.478884	10.088690	13.577261
C	9.749659	12.647131	10.418312	H	15.691456	8.764800	13.540319
C	9.809176	15.087676	10.140110	H	14.986796	9.289621	15.084850

GO-CF<sub>3</sub>\_DK-keto (above)

C	19.103014	11.103747	10.275498	C	8.469110	15.029574	10.273832
C	18.450140	12.302492	10.453691	C	7.762107	13.833723	10.251256
C	19.193819	13.570908	10.435698	C	8.411684	12.593586	10.402346
C	20.584526	13.573184	10.229510	C	10.373741	6.488476	9.415847
C	21.341450	12.313090	10.218498	C	9.650478	7.691245	9.718845
C	20.565603	11.032169	10.198798	C	8.322138	10.152814	10.205963
C	18.505428	14.821766	10.532652	C	8.267163	7.744642	9.629206
C	21.310369	14.774184	10.026750	C	7.511864	8.946099	9.882402
C	20.634670	16.000874	10.151175	C	7.688036	11.380698	10.272270
C	19.244673	16.047682	10.394829	C	14.661509	6.348118	9.468646
C	21.424631	17.242123	10.110970	C	12.504387	5.269404	9.078453
C	22.775633	17.192928	9.532431	C	13.872077	5.239398	9.051281
C	23.419409	15.976230	9.434921	C	7.619259	16.246296	10.113932
C	22.731850	14.747669	9.744821	C	9.620654	5.262837	8.999445
C	23.415073	13.528243	9.641100	C	17.184624	17.575623	12.440896
C	22.716824	12.310076	9.686754	C	12.970961	11.221805	14.797451

C	17.011518	12.315411	10.609694	C	14.139477	12.047657	14.372015
C	16.355278	13.586137	11.066899	C	14.120073	13.534313	14.766134
C	17.085182	14.859643	10.688939	C	14.601605	13.722239	16.184519
C	16.373798	16.047939	10.674240	C	15.986325	14.435125	16.318762
C	17.111416	17.355186	10.854515	O	26.691854	13.015759	11.168974
C	18.561512	17.312317	10.419250	O	24.803473	14.056875	11.880616
C	20.680904	18.551174	10.099931	O	16.534145	13.622533	12.533917
C	19.209965	18.501516	10.153503	O	21.322474	18.067917	11.318103
C	24.792765	15.926328	8.945642	O	21.243938	22.038113	8.972122
C	25.485113	14.764839	8.945081	O	18.458986	5.759195	7.720048
C	21.353775	19.726809	9.493049	O	19.922228	5.834250	9.445730
C	23.419235	18.421764	9.107624	O	14.398241	7.809252	11.440063
C	22.666496	19.647121	9.107916	O	21.234867	11.488850	11.432514
C	18.496471	19.735800	9.963968	O	14.236068	19.586275	9.814885
C	17.099592	19.718014	10.005779	O	26.617046	17.154675	7.978080
C	16.367756	18.563890	10.305091	O	10.350168	11.149532	12.422665
C	14.944778	16.063787	10.668775	O	6.505581	16.239191	9.607963
C	14.212034	14.878992	10.815706	O	8.156940	17.395437	10.628862
C	14.863642	13.630792	10.820046	O	9.673255	4.752194	7.891792
C	16.256859	11.155068	10.487783	O	8.865701	4.752288	10.012111
C	16.903494	9.897974	10.248955	O	18.192423	17.864641	13.048103
C	18.393785	9.794317	10.433327	O	15.971542	17.410830	13.026761
C	21.175507	9.867831	9.533861	O	6.263000	8.978863	9.824476
C	22.510847	9.926083	9.142145	O	25.079546	9.963016	8.168169
C	23.283342	11.102491	9.235079	O	18.486797	9.416409	11.867400
C	19.023327	8.655377	9.646043	O	12.599139	15.112553	12.579289
C	20.361948	8.751065	9.272603	O	15.073095	11.594908	13.713194
C	24.653994	11.141011	8.727106	O	14.007553	13.364682	17.183409
C	25.412212	12.254604	8.801743	H	26.524263	14.764285	8.604353
C	25.472010	17.182404	8.469486	H	23.159786	20.542662	8.726248
C	24.715727	18.402454	8.619486	H	16.591955	20.645452	9.717377
C	20.568150	20.922094	9.373701	H	22.963680	9.045097	8.685064
C	19.212934	20.919710	9.621461	H	18.645050	21.846825	9.493035
C	14.976254	18.499771	10.180097	H	25.199619	19.325720	8.294288
C	14.232680	17.311934	10.404551	H	26.449047	12.256867	8.460125
C	14.125617	12.447414	10.709770	H	20.832987	7.910782	8.760057
C	14.798512	11.193069	10.543751	H	25.309607	14.053406	12.722256
C	24.917931	13.491040	9.501810	H	16.126497	12.794352	12.913184
C	25.588446	13.470035	10.948347	H	20.623413	22.786156	8.894579
C	18.231453	7.513948	9.370960	H	16.511559	5.482328	8.925594
C	16.201967	8.734051	10.055868	H	12.349632	18.221220	9.933996
C	14.055784	10.025742	10.419297	H	20.244631	5.050798	8.948593
C	12.674233	12.478892	10.720522	H	6.681907	13.864927	10.100855
C	12.730275	14.952658	11.091988	H	14.818969	20.358391	9.698910
C	12.850565	17.305550	10.250961	H	6.604396	11.402132	10.127142
C	16.840534	7.510438	9.619355	H	14.388315	4.350320	8.680634
C	14.754903	8.734317	10.353575	H	11.947452	4.396394	8.738833
C	12.616833	10.038383	10.434847	H	10.446507	10.198562	12.632538
C	11.951666	11.244343	10.628829	H	7.474515	18.085136	10.479469
C	11.985461	13.690861	10.800816	H	8.398734	3.969924	9.644136
C	12.071480	16.156467	10.478672	H	16.117502	17.495365	13.993992
C	10.703129	16.164217	10.267123	H	10.242019	17.099047	9.952497
C	13.954736	7.496058	10.077100	H	7.683432	6.861729	9.368817
C	16.031757	6.370382	9.336733	H	26.011045	10.057210	7.895971
C	18.849262	6.306993	8.741425	H	19.390009	9.639802	12.172571

C	10.556458	13.746253	10.642451	H	13.012571	15.974096	12.795066
C	10.477349	11.250484	10.928334	H	13.179318	10.155784	14.650966
C	11.856502	8.816316	10.169283	H	12.700249	11.441794	15.841551
C	12.494707	7.619235	9.884115	H	12.107849	11.516460	14.170544
C	11.765709	6.447120	9.455344	H	13.081778	13.892829	14.711002
C	10.416003	8.881974	10.090290	H	14.738482	14.093502	14.053311
C	9.739265	10.066270	10.354786	F	15.915552	15.684625	15.743141
C	9.812008	12.564817	10.621771	F	16.364248	14.592983	17.599390
C	9.891027	15.014724	10.427893	F	16.948221	13.735779	15.663587
GO-CF <sub>3</sub> DK-enol (above)							
C	19.038376	11.135650	10.228582	C	8.438540	15.134546	10.081302
C	18.390642	12.341475	10.387562	C	7.724533	13.941212	10.038286
C	19.145466	13.604872	10.380880	C	8.361112	12.696666	10.199698
C	20.540293	13.596087	10.205475	C	10.287515	6.555459	9.339334
C	21.285372	12.328814	10.203346	C	9.569242	7.768268	9.615651
C	20.500912	11.055269	10.171838	C	8.254608	10.250637	10.047298
C	18.462742	14.860966	10.465639	C	8.185729	7.828190	9.531799
C	21.282639	14.791761	10.030980	C	7.436941	9.037257	9.773191
C	20.613800	16.022974	10.144861	C	7.630546	11.485112	10.083198
C	19.216248	16.081371	10.347393	C	14.577243	6.400266	9.401501
C	21.413088	17.258181	10.135345	C	12.416508	5.325706	9.015055
C	22.788565	17.201630	9.618624	C	13.784137	5.291439	8.990791
C	23.424353	15.979641	9.529627	C	7.596746	16.356396	9.911971
C	22.712059	14.753366	9.789330	C	9.531162	5.319038	8.965450
C	23.381628	13.527118	9.677528	C	17.100796	17.748819	12.293185
C	22.667446	12.316818	9.690811	C	12.053338	12.777302	14.667010
C	16.949877	12.364210	10.525617	C	13.532704	12.781960	14.790079
C	16.283140	13.642329	10.938711	C	14.278274	13.900002	15.163862
C	17.038719	14.908885	10.589686	C	15.681431	13.777550	15.297824
C	16.340536	16.109400	10.543484	C	16.518009	15.002281	15.733551
C	17.081264	17.411812	10.720995	O	26.652834	12.958059	11.225041
C	18.542046	17.350107	10.334660	O	24.713409	13.870974	11.976334
C	20.676252	18.574732	10.085073	O	16.255096	13.644848	12.430754
C	19.205643	18.531746	10.070619	O	21.257259	18.089617	11.331177
C	24.817739	15.923902	9.100845	O	21.306055	22.045876	8.945006
C	25.489983	14.750921	9.077999	O	18.395456	5.782323	7.698367
C	21.384045	19.743269	9.505956	O	19.831125	5.852949	9.447342
C	23.461811	18.429895	9.238987	O	14.304543	7.875498	11.358898
C	22.717014	19.658503	9.198650	O	21.155493	11.505528	11.417187
C	18.503622	19.758791	9.804460	O	14.236515	19.654720	9.628044
C	17.106134	19.743608	9.781782	O	26.722498	17.158131	8.313004
C	16.358315	18.611576	10.117040	O	10.264844	11.266952	12.243384
C	14.916362	16.135450	10.506781	O	6.495309	16.356905	9.379643
C	14.174478	14.950473	10.623981	O	8.126010	17.499470	10.446943
C	14.807312	13.697330	10.636984	O	9.589382	4.762495	7.880188
C	16.190926	11.204543	10.407323	O	8.768302	4.852432	9.993350
C	16.833315	9.942717	10.183806	O	17.964260	18.405756	12.834736
C	18.319567	9.831659	10.387787	O	16.011106	17.254190	12.915623
C	21.110567	9.885448	9.514927	O	6.186861	9.067445	9.752018
C	22.447998	9.937434	9.130340	O	25.014875	9.970822	8.151527
C	23.227184	11.108978	9.232923	O	18.389315	9.469083	11.828475
C	18.950804	8.683941	9.616087	O	12.611140	15.222839	12.408963
C	20.293442	8.771331	9.253312	O	14.128044	11.631905	14.527154

C	24.600864	11.141973	8.732787	O	16.336285	12.716491	15.112214
C	25.370720	12.245616	8.834067	H	26.542692	14.747522	8.781921
C	25.541412	17.184536	8.710205	H	23.2339 00	20.550417	8.840562
C	24.784042	18.406761	8.825818	H	16.613686	20.655645	9.426583
C	20.606876	20.934521	9.317537	H	22.899117	9.055140	8.674011
C	19.237469	20.932493	9.470324	H	18.678524	21.854874	9.283041
C	14.963535	18.564587	10.007996	H	25.292479	19.330486	8.541909
C	14.209594	17.389257	10.260745	H	26.409534	12.245381	8.498446
C	14.067160	12.513824	10.557052	H	20.763823	7.925893	8.748437
C	14.733762	11.252358	10.439365	H	25.208771	13.830321	12.823549
C	24.885469	13.468142	9.566582	H	17.118759	13.322719	12.761919
C	25.534058	13.380618	11.019362	H	20.690321	22.789968	8.811171
C	18.155472	7.545133	9.339233	H	16.428310	5.519023	8.887085
C	16.126781	8.781240	9.990512	H	12.327146	18.320232	9.838339
C	13.983935	10.087520	10.318426	H	20.154932	5.064025	8.959773
C	12.617818	12.552688	10.550249	H	6.647208	13.981226	9.869727
C	12.701764	15.026972	10.926453	H	14.821196	20.430738	9.553432
C	12.825845	17.397930	10.139139	H	6.547137	11.512028	9.937326
C	16.761839	7.550215	9.570500	H	14.297966	4.396505	8.631251
C	14.676304	8.791723	10.271286	H	11.858172	4.450167	8.684813
C	12.546524	10.109414	10.305848	H	10.555511	10.366816	12.496679
C	11.888851	11.324306	10.471506	H	7.450467	18.193432	10.286530
C	11.941969	13.773495	10.619869	H	8.300525	4.057729	9.654140
C	12.042149	16.251638	10.360062	H	16.083725	17.476471	13.869815
C	10.676785	16.265339	10.142497	H	10.220367	17.208019	9.845239
C	13.871284	7.556283	9.994309	H	7.594898	6.942918	9.296997
C	15.948903	6.413407	9.284860	H	25.948599	10.059116	7.885190
C	18.773762	6.330836	8.723604	H	19.317709	9.588565	12.116780
C	10.511242	13.837716	10.459209	H	13.401286	14.788555	12.794467
C	10.412005	11.344596	10.754127	H	11.633292	12.050597	15.380590
C	11.780403	8.890127	10.047976	H	13.776056	14.841635	15.369607
C	12.413586	7.685513	9.787233	H	11.629192	13.768925	14.857865
C	11.680182	6.510466	9.375570	H	11.745948	12.444993	13.662429
C	10.340816	8.963308	9.958164	H	15.136410	11.792372	14.675342
C	9.671054	10.156651	10.194605	F	15.793997	16.174652	15.721979
C	9.760015	12.661925	10.431339	F	16.984127	14.834651	16.998636
C	9.856535	15.112592	10.260110	F	17.586346	15.188016	14.916745

GO-MAA-keto (above)

C	19.061386	11.068879	10.282225	C	7.712171	13.746196	10.107909
C	18.402758	12.264870	10.461917	C	8.365437	12.509245	10.262653
C	19.142767	13.535567	10.458439	C	10.359422	6.372082	9.495758
C	20.536787	13.542903	10.269415	C	9.629974	7.584613	9.742876
C	21.295879	12.284192	10.249815	C	8.290115	10.060756	10.129341
C	20.524220	11.002756	10.211476	C	8.246769	7.629632	9.649092
C	18.447592	14.782857	10.550341	C	7.486754	8.838365	9.850897
C	21.264193	14.746976	10.094184	C	7.650189	11.287792	10.159284
C	20.582121	15.970398	10.217236	C	14.650976	6.274348	9.509317
C	19.185987	16.011620	10.425566	C	12.500360	5.159031	9.185185
C	21.369043	17.214607	10.216639	C	13.868036	5.143763	9.139596
C	22.739408	17.176855	9.683934	C	7.546150	16.157795	9.993859
C	23.386942	15.962269	9.577897	C	9.612242	5.118997	9.160412
C	22.691917	14.726461	9.838819	C	17.048334	17.442793	12.409076
C	23.374310	13.509089	9.712725	C	12.356636	13.027865	14.905243

C	22.673399	12.291031	9.724511	C	13.812024	12.938302	14.585663
C	16.962725	12.272016	10.602757	C	14.800345	13.743879	15.444956
C	16.286835	13.538954	11.042127	C	14.908069	15.204810	15.040292
C	17.024029	14.814062	10.688828	C	17.359388	15.088236	15.309468
C	16.307665	16.000586	10.639258	O	26.665956	12.963153	11.223212
C	17.037064	17.317383	10.813435	O	24.731655	13.865973	11.998075
C	18.499670	17.273804	10.430660	O	16.396049	13.550154	12.529025
C	20.622576	18.522467	10.196102	O	21.221636	18.024876	11.431457
C	19.151501	18.467470	10.191718	O	21.217300	22.030075	9.155489
C	24.774910	15.924216	9.129390	O	18.438725	5.714430	7.725221
C	25.461399	14.759782	9.094697	O	19.917276	5.809159	9.436931
C	21.313599	19.709301	9.634001	O	14.378916	7.777556	11.448063
C	23.395357	18.415075	9.307135	O	21.186602	11.445660	11.455557
C	22.641006	19.639139	9.300719	O	14.184728	19.517374	9.662922
C	18.437590	19.696362	9.976931	O	26.649458	17.181206	8.307084
C	17.039150	19.667240	9.952771	O	10.311696	11.144760	12.306789
C	16.304708	18.510147	10.230161	O	6.406376	16.134192	9.549162
C	14.879472	16.015720	10.607279	O	8.100817	17.322586	10.451318
C	14.151195	14.827897	10.738095	O	9.667461	4.532984	8.090537
C	14.807077	13.581469	10.747193	O	8.859747	4.673499	10.205677
C	16.215588	11.107688	10.464876	O	18.031012	17.225258	13.090033
C	16.869423	9.853014	10.235966	O	15.824649	17.732626	12.886839
C	18.357561	9.755454	10.430683	O	6.237699	8.862050	9.789498
C	21.139345	9.846875	9.535592	O	25.032099	9.980539	8.147760
C	22.473083	9.915318	9.141851	O	18.443104	9.376577	11.866895
C	23.241360	11.093323	9.250700	O	12.478882	14.965583	12.453356
C	18.994537	8.621184	9.643154	O	14.257982	12.219560	13.692298
C	20.331507	8.727435	9.267420	O	13.949483	15.892165	14.717937
C	24.610445	11.144069	8.739697	O	16.118362	15.812010	15.093214
C	25.369621	12.254926	8.841025	H	26.509907	14.769409	8.784107
C	25.477030	17.194334	8.730313	H	23.147022	20.541737	8.953897
C	24.710438	18.408113	8.870488	H	16.538416	20.591736	9.643499
C	20.527672	20.902843	9.501040	H	22.928539	9.041961	8.672818
C	19.161945	20.889088	9.681051	H	18.595406	21.814817	9.537342
C	14.915807	18.440567	10.070210	H	25.205076	19.339186	8.586203
C	14.168256	17.258907	10.313414	H	26.405586	12.267240	8.496785
C	14.078093	12.395892	10.619781	H	20.806664	7.892841	8.749384
C	14.757332	11.140965	10.490728	H	25.239697	13.826268	12.837691
C	24.877920	13.467805	9.585625	H	15.727650	12.898488	12.875143
C	25.542931	13.380764	11.029648	H	20.596504	22.775198	9.055766
C	18.209949	7.473508	9.369925	H	16.505541	5.414820	8.970708
C	16.174547	8.684359	10.044798	H	12.286418	18.164310	9.835220
C	14.020812	9.968685	10.374278	H	20.241903	5.027418	8.938658
C	12.627971	12.419623	10.592927	H	6.630920	13.773990	9.963588
C	12.663662	14.886877	10.987774	H	14.769599	20.288301	9.549504
C	12.787528	17.250483	10.157249	H	6.566265	11.299064	10.015171
C	16.819960	7.460485	9.621459	H	14.389260	4.247463	8.794013
C	14.727110	8.679867	10.338509	H	11.949503	4.267632	8.886059
C	12.582212	9.972990	10.369474	H	10.701143	10.290358	12.583938
C	11.912354	11.181538	10.519423	H	7.404652	18.002731	10.324347
C	11.932727	13.625230	10.646914	H	8.398182	3.865314	9.890623
C	12.009831	16.099524	10.382090	H	15.813062	17.502069	13.847365
C	10.644784	16.101934	10.150805	H	10.182408	17.038120	9.843124
C	13.936763	7.431679	10.091356	H	7.666054	6.734744	9.425341
C	16.019541	6.307868	9.363757	H	25.963551	10.079691	7.877466

C	18.833271	6.270274	8.740747	H	19.365616	9.536019	12.154053
C	10.503755	13.676522	10.485973	H	13.072125	15.652356	12.828848
C	10.438643	11.190063	10.816439	H	11.758774	12.511318	14.145170
C	11.829163	8.739132	10.140819	H	12.178505	12.587120	15.901499
C	12.474955	7.537283	9.898652	H	12.064185	14.087110	14.961734
C	11.752458	6.343249	9.523496	H	15.769629	13.234711	15.407353
C	10.388618	8.794225	10.060537	H	14.451157	13.749704	16.491745
C	9.706957	9.984089	10.281034	H	17.367310	14.625805	16.306530
C	9.766371	12.492651	10.476908	H	17.501713	14.346950	14.511298
C	9.834485	14.944345	10.283898	H	18.138699	15.853026	15.236462
C	8.411754	14.948785	10.132990				
GO-MAA-enol (above)							
C	19.006306	11.148549	10.388661	C	7.675857	13.885193	9.987345
C	18.346615	12.351965	10.498837	C	8.319180	12.648543	10.177774
C	19.089144	13.621012	10.447345	C	10.287026	6.496112	9.506734
C	20.481934	13.620281	10.258856	C	9.559041	7.713747	9.731022
C	21.241446	12.363478	10.290977	C	8.226040	10.199892	10.066377
C	20.470812	11.076682	10.336624	C	8.178027	7.764675	9.611526
C	18.399519	14.873850	10.500395	C	7.419362	8.977246	9.798255
C	21.211958	14.818061	10.050782	C	7.596634	11.431234	10.065738
C	20.538166	16.046957	10.160608	C	14.574692	6.366945	9.634434
C	19.144251	16.098156	10.371828	C	12.425857	5.269211	9.250435
C	21.334438	17.284552	10.152922	C	13.793867	5.242605	9.244166
C	22.697006	17.234369	9.601756	C	7.520986	16.291330	9.824588
C	23.333372	16.014278	9.495152	C	9.542253	5.242048	9.168156
C	22.635942	14.786237	9.785979	C	17.029524	17.526283	12.369319
C	23.313719	13.563184	9.685737	C	12.761381	11.934957	14.425436
C	22.613358	12.347065	9.753302	C	14.219130	11.968522	14.720412
C	16.902807	12.368726	10.629816	C	14.910508	13.117646	15.035954
C	16.234692	13.656775	11.009136	C	16.338625	13.062788	15.240551
C	16.977308	14.915714	10.618202	C	18.348680	14.303511	15.400398
C	16.266857	16.106789	10.574078	O	26.595663	13.013741	11.192171
C	17.004461	17.413668	10.775567	O	24.716185	14.056170	11.925668
C	18.467005	17.364622	10.385589	O	16.382727	13.749994	12.486950
C	20.599241	18.597094	10.145779	O	21.205917	18.089399	11.373944
C	19.126919	18.554976	10.154467	O	21.217646	22.110001	9.142640
C	24.711906	15.960399	9.021553	O	18.393486	5.807466	7.896208
C	25.392923	14.791991	9.002090	O	19.802530	5.835309	9.668547
C	21.295343	19.780704	9.582657	O	14.264346	7.884711	11.554395
C	23.356701	18.465237	9.208714	O	21.135595	11.590174	11.534623
C	22.615030	19.697901	9.222807	O	14.165276	19.638285	9.641503
C	18.422174	19.792915	9.960116	O	26.567390	17.192034	8.121346
C	17.023483	19.775852	9.944523	O	10.173495	11.270345	12.285862
C	16.280315	18.619795	10.206646	O	6.390999	16.254940	9.356473
C	14.842945	16.125763	10.551216	O	8.068558	17.471785	10.249652
C	14.106537	14.940376	10.699235	O	9.620624	4.641442	8.107862
C	14.753282	13.692504	10.739048	O	8.765330	4.813453	10.202162
C	16.150969	11.203105	10.547090	O	18.008204	17.330687	13.057952
C	16.805304	9.938108	10.365644	O	15.802208	17.819229	12.874042
C	18.294340	9.842925	10.577546	O	6.170633	9.004004	9.738468
C	21.082903	9.894211	9.704830	O	24.944317	9.984365	8.214504
C	22.411434	9.946931	9.288455	O	18.485596	9.458395	11.994987
C	23.178310	11.129972	9.326048	O	12.500862	15.140713	12.461864

C	18.930660	8.683463	9.828142	O	14.831429	10.784950	14.633142
C	20.272301	8.770445	9.469192	O	17.014746	12.010067	15.175838
C	24.535265	11.164664	8.780809	O	16.904434	14.270422	15.459825
C	25.294003	12.279835	8.827741	H	26.434616	14.789214	8.669184
C	25.410625	17.219664	8.584553	H	23.124378	20.597668	8.873314
C	24.660915	18.442991	8.741604	H	16.528135	20.709000	9.652639
C	20.520237	20.984818	9.477843	H	22.860550	9.054406	8.850354
C	19.156624	20.982405	9.674175	H	18.598604	21.916142	9.549969
C	14.892375	18.555641	10.040078	H	25.158916	19.367516	8.442186
C	14.137535	17.374971	10.274659	H	26.321348	12.281853	8.458565
C	14.017002	12.503027	10.671176	H	20.745121	7.919516	8.975617
C	14.691755	11.242566	10.574151	H	25.226381	14.039026	12.764561
C	24.815346	13.515878	9.540031	H	15.542808	13.451650	12.907075
C	25.493265	13.475362	10.983128	H	20.603735	22.862783	9.058848
C	18.140587	7.541757	9.564074	H	16.436766	5.488568	9.155867
C	16.102232	8.770436	10.188730	H	12.255315	18.283407	9.803362
C	13.949684	10.072078	10.463341	H	20.131054	5.052569	9.174122
C	12.566481	12.536486	10.636853	H	6.600926	13.914577	9.802835
C	12.625309	15.012707	10.974159	H	14.755619	20.403536	9.517088
C	12.756098	17.370228	10.128073	H	6.516473	11.450878	9.895962
C	16.746780	7.538156	9.795954	H	14.317100	4.341364	8.915072
C	14.649075	8.778774	10.452098	H	11.876348	4.382287	8.936494
C	12.512074	10.087236	10.426128	H	10.355114	10.346382	12.552911
C	11.845069	11.301341	10.556077	H	7.376171	18.146856	10.081110
C	11.879274	13.751998	10.669874	H	8.307912	4.002237	9.888842
C	11.973903	16.221085	10.359353	H	15.897973	17.783377	13.850183
C	10.612770	16.227936	10.108063	H	10.162382	17.163099	9.780678
C	13.855066	7.533194	10.190798	H	7.597145	6.870366	9.386029
C	15.946959	6.388266	9.528775	H	25.870382	10.074152	7.922971
C	18.761614	6.332041	8.937188	H	18.128759	10.183956	12.549082
C	10.455199	13.808523	10.466866	H	12.978112	15.960239	12.707194
C	10.361159	11.319126	10.804340	H	12.236311	11.349345	15.196241
C	11.757037	8.857527	10.179565	H	14.388994	14.069378	15.102339
C	12.399965	7.650187	9.958228	H	12.333526	12.942364	14.371828
C	11.678926	6.459623	9.566614	H	12.583980	11.431736	13.463942
C	10.318926	8.921336	10.057940	H	15.812282	10.972182	14.849037
C	9.639472	10.116814	10.249072	H	18.785660	13.696397	16.205067
C	9.711374	12.626396	10.438733	H	18.687674	13.923864	14.426202
C	9.795228	15.075529	10.228276	H	18.617243	15.359410	15.510437
C	8.378551	15.084539	10.022293				

GO-DMM-keto (above)

C	19.032293	11.176253	10.444770	C	7.721860	13.977970	9.972965
C	18.382723	12.382836	10.577738	C	8.357008	12.736036	10.170902
C	19.133213	13.645385	10.538548	C	10.289912	6.566485	9.546287
C	20.524639	13.638542	10.334272	C	9.568312	7.789475	9.760056
C	21.277519	12.377162	10.339182	C	8.249973	10.286218	10.078040
C	20.495275	11.092092	10.377482	C	8.188232	7.848875	9.634893
C	18.448605	14.902702	10.602036	C	7.436798	9.066964	9.814009
C	21.259384	14.833675	10.120066	C	7.628304	11.521524	10.063965
C	20.592068	16.066906	10.231811	C	14.574913	6.413001	9.691244
C	19.199081	16.125256	10.453068	C	12.420205	5.319595	9.326170
C	21.394966	17.301043	10.209459	C	13.788107	5.285744	9.321454
C	22.754700	17.242207	9.651797	C	7.600413	16.393127	9.824900



C	23.382771	16.018263	9.541585	C	9.539257	5.321622	9.188077
C	22.679575	14.794861	9.838151	C	17.070648	17.646471	12.402699
C	23.349274	13.567547	9.722105	C	16.149973	11.217191	14.508394
C	22.641594	12.357303	9.783403	C	17.211514	11.814939	15.409398
C	16.939014	12.406839	10.703012	C	18.250221	12.591898	14.614552
C	16.261410	13.690346	11.087637	C	19.329103	14.675541	14.379167
C	17.026213	14.950249	10.733451	C	13.806633	11.110780	14.109006
C	16.323124	16.150976	10.652893	O	26.638918	13.002866	11.204947
C	17.063499	17.463242	10.821615	O	24.763756	14.039596	11.956681
C	18.529819	17.396465	10.446318	O	16.300884	13.682744	12.592954
C	20.666628	18.619009	10.192465	O	21.272287	18.118227	11.423453
C	19.195139	18.581656	10.197349	O	21.301020	22.120150	9.151035
C	24.757071	15.956830	9.054615	O	18.364506	5.832019	7.900732
C	25.431458	14.785188	9.027603	O	19.805050	5.877304	9.646837
C	21.367672	19.794809	9.618382	O	14.277530	7.958251	11.595123
C	23.420347	18.467041	9.249343	O	21.187365	11.580407	11.562788
C	22.686329	19.703424	9.258702	O	14.244781	19.677223	9.616879
C	18.496563	19.818048	9.972446	O	26.612854	17.173939	8.134226
C	17.098846	19.803875	9.933638	O	10.215398	11.366677	12.293245
C	16.350550	18.655212	10.207232	O	6.528819	16.404318	9.235394
C	14.903467	16.176979	10.585484	O	8.101604	17.525116	10.411038
C	14.156692	14.991662	10.704783	O	9.613710	4.742766	8.115650
C	14.794299	13.741020	10.747705	O	8.760238	4.877082	10.213708
C	16.179552	11.249899	10.573903	O	18.030582	17.442827	13.116673
C	16.824301	9.982718	10.379845	O	15.851347	18.015305	12.877712
C	18.310911	9.866357	10.602808	O	6.188386	9.100588	9.750926
C	21.090988	9.920087	9.710189	O	24.950850	9.990144	8.214030
C	22.418234	9.966689	9.286833	O	18.503233	9.442271	11.986715
C	23.195686	11.140118	9.338778	O	12.556650	15.197230	12.461009
C	18.934891	8.721321	9.817970	O	16.362167	10.449447	13.580483
C	20.273706	8.805893	9.453501	O	18.905954	12.135142	13.697683
C	24.551249	11.168547	8.791150	O	18.368469	13.854012	15.090070
C	25.319347	12.276697	8.847449	O	14.919248	11.616890	14.890872
C	25.461016	17.210648	8.609521	H	26.470079	14.776948	8.685246
C	24.720695	18.437616	8.771929	H	23.198568	20.597935	8.900146
C	20.598757	21.000702	9.495279	H	16.610067	20.732044	9.615994
C	19.234203	21.003288	9.678862	H	22.854910	9.077212	8.830479
C	14.964077	18.596767	10.035538	H	18.677938	21.935272	9.535518
C	14.204289	17.424290	10.285448	H	25.219387	19.359343	8.465352
C	14.051516	12.556539	10.660987	H	26.346954	12.273739	8.478910
C	14.721153	11.295797	10.576342	H	20.741785	7.960806	8.945358
C	24.849670	13.511816	9.566454	H	25.281687	14.017366	12.790746
C	25.534651	13.464246	11.004963	H	15.499880	14.164236	12.889642
C	18.140724	7.582050	9.557236	H	20.688574	22.872398	9.052956
C	16.114183	8.818987	10.204447	H	16.429352	5.526908	9.197151
C	13.971415	10.129042	10.469931	H	12.333549	18.340935	9.788224
C	12.603431	12.598366	10.621542	H	20.124050	5.090798	9.152325
C	12.674228	15.072797	10.968843	H	6.648579	14.013512	9.779350
C	12.824014	17.426682	10.125540	H	14.840494	20.436878	9.484342
C	16.750475	7.583231	9.810141	H	6.549241	11.545312	9.888008
C	14.663544	8.833651	10.475325	H	14.307078	4.377391	9.005239
C	12.534877	10.150512	10.434343	H	11.866259	4.430483	9.025801
C	11.874076	11.369057	10.553385	H	10.447088	10.458304	12.574398
C	11.923109	13.818298	10.659374	H	7.435616	18.223040	10.229498
C	12.030867	16.285509	10.356450	H	8.296658	4.075868	9.884107

C	10.668404	16.300922	10.109042	H	15.940681	18.049883	13.854214
C	13.862565	7.589356	10.235924	H	10.221541	17.239399	9.783836
C	15.945707	6.431432	9.566862	H	7.602109	6.957238	9.411994
C	18.750738	6.368063	8.929779	H	25.876793	10.076502	7.921144
C	10.500392	13.882071	10.462956	H	17.925354	9.986930	12.580566
C	10.392152	11.397470	10.810052	H	12.714835	16.139475	12.673319
C	11.772063	8.922843	10.205439	H	17.740202	10.973010	15.884069
C	12.408010	7.709270	10.002384	H	16.756824	12.441321	16.183266
C	11.680332	6.519293	9.621551	H	20.315088	14.191428	14.375080
C	10.334257	8.994065	10.083360	H	18.991825	14.829247	13.346928
C	9.662009	10.194740	10.266779	H	19.351923	15.630672	14.911982
C	9.747784	12.705287	10.436552	H	13.724112	11.687773	13.179031
C	9.847902	15.152208	10.230034	H	13.950085	10.048331	13.871318
C	8.433710	15.170297	10.019539	H	12.917967	11.270303	14.728242
GO-DMM-enol (above)							
C	19.090473	11.041481	10.289118	C	7.784678	13.804538	9.842266
C	18.434034	12.239147	10.465389	C	8.415552	12.558519	10.010960
C	19.174095	13.508273	10.464756	C	10.394517	6.448123	9.081779
C	20.564941	13.515206	10.255488	C	9.662504	7.653071	9.353525
C	21.326488	12.258582	10.241643	C	8.324110	10.119678	9.788820
C	20.554533	10.973779	10.225467	C	8.284425	7.714209	9.202852
C	18.484116	14.755255	10.588457	C	7.522837	8.916261	9.436184
C	21.286987	14.718837	10.062925	C	7.694431	11.351588	9.829065
C	20.610861	15.942137	10.213331	C	14.674264	6.289086	9.332001
C	19.224821	15.983724	10.474531	C	12.532435	5.218769	8.846448
C	21.402304	17.183775	10.189747	C	13.899416	5.183075	8.881642
C	22.741499	17.144924	9.582567	C	7.652306	16.216837	9.732185
C	23.386271	15.931314	9.460258	C	9.659321	5.228125	8.621968
C	22.706436	14.698493	9.769088	C	17.208462	17.288214	12.623487
C	23.393909	13.483301	9.655910	C	14.558371	13.340658	14.851502
C	22.701828	12.261160	9.708449	C	14.782799	14.727821	15.056515
C	16.992136	12.249330	10.600863	C	16.009785	15.073136	15.589233
C	16.326651	13.505193	11.080690	C	17.622375	16.664898	16.356846
C	17.065277	14.789122	10.758700	C	13.113043	11.609580	14.058299
C	16.355715	15.980453	10.796599	O	26.685083	12.992644	11.158586
C	17.108101	17.278076	11.024061	O	24.804667	14.041496	11.879192
C	18.547394	17.248394	10.556722	O	16.477348	13.492764	12.563809
C	20.665236	18.491772	10.229750	O	21.334805	17.978415	11.423749
C	19.195494	18.445364	10.322418	O	21.209555	22.005610	9.177076
C	24.751953	15.889555	8.949701	O	18.578773	5.649541	7.797368
C	25.450050	14.731337	8.938085	O	19.915678	5.759266	9.622332
C	21.324919	19.680901	9.634053	O	14.338118	7.747401	11.291105
C	23.375189	18.380423	9.162556	O	21.218027	11.438329	11.457670
C	22.625341	19.606426	9.206802	O	14.227839	19.586857	10.217651
C	18.485437	19.688456	10.204190	O	26.552452	17.131239	7.955296
C	17.089455	19.676434	10.295156	O	10.234617	11.071005	12.108382
C	16.361979	18.515131	10.567205	O	6.560140	16.205364	9.180236
C	14.926579	16.003490	10.791494	O	8.168953	17.373053	10.250167
C	14.189336	14.812935	10.844871	O	9.769269	4.722034	7.516334
C	14.840325	13.563874	10.805360	O	8.849264	4.716452	9.590709
C	16.239172	11.090981	10.441178	O	18.225092	17.004370	13.226839
C	16.892334	9.835068	10.202662	O	16.026251	17.570353	13.197175
C	18.376093	9.732984	10.435205	O	6.275730	8.950521	9.346095

C	21.175562	9.807750	9.573222	O	25.067616	9.923821	8.180750
C	22.509771	9.872375	9.180750	O	18.417999	9.372004	11.878205
C	23.274136	11.055632	9.260347	O	12.458160	15.055443	12.501117
C	19.027481	8.587886	9.678572	O	15.378000	12.429014	15.166245
C	20.370567	8.682102	9.324103	O	16.910051	14.195384	15.963926
C	24.640339	11.100999	8.740719	O	16.335295	16.377108	15.738469
C	25.392014	12.219566	8.803569	O	13.378204	13.021624	14.258606
C	25.416710	17.151066	8.468584	H	26.484772	14.735706	8.583888
C	24.660784	18.367828	8.645350	H	23.110439	20.509369	8.831750
C	20.542046	20.881790	9.573487	H	16.578880	20.614237	10.048798
C	19.196823	20.878996	9.871889	H	22.968340	8.990601	8.730687
C	14.965537	18.469162	10.473217	H	18.630239	21.812382	9.791116
C	14.222309	17.267969	10.591906	H	25.137665	19.295597	8.322027
C	14.105191	12.385836	10.622436	H	26.424921	12.227966	8.450130
C	14.779650	11.131680	10.453133	H	20.849569	7.836773	8.826311
C	24.896219	13.455112	9.503963	H	25.320831	14.045479	12.714643
C	25.579868	13.445678	10.943948	H	16.310005	12.578495	12.874199
C	18.246511	7.440284	9.395645	H	20.589243	22.756727	9.137209
C	16.196363	8.673274	9.981139	H	16.543987	5.414598	8.875902
C	14.038965	9.967773	10.275077	H	12.363605	18.207850	10.091621
C	12.653675	12.417356	10.561840	H	20.269854	4.962788	9.169437
C	12.691682	14.874666	11.055737	H	6.717075	13.844944	9.620889
C	12.850392	17.273149	10.372678	H	14.807436	20.369965	10.215341
C	16.848043	7.442883	9.579228	H	6.619362	11.380121	9.630781
C	14.738379	8.675145	10.220790	H	14.428295	4.291243	8.536496
C	12.601077	9.982574	10.225853	H	11.988273	4.347547	8.482388
C	11.932995	11.188381	10.407385	H	10.285402	10.113729	12.305159
C	11.965379	13.629620	10.644923	H	7.493008	18.059774	10.063118
C	12.068118	16.111923	10.468205	H	8.398540	3.938604	9.194108
C	10.722520	16.128288	10.151982	H	16.095549	17.318487	14.158063
C	13.946563	7.439998	9.910038	H	10.284492	17.078148	9.851349
C	16.048618	6.305182	9.262913	H	7.708416	6.834754	8.915151
C	18.898022	6.218011	8.831861	H	25.996655	10.022079	7.901714
C	10.544369	13.696020	10.406915	H	19.338470	9.503864	12.185368
C	10.443757	11.196396	10.627908	H	12.774643	14.251135	12.976885
C	11.850065	8.765944	9.912848	H	14.064488	15.475865	14.735067
C	12.496328	7.567539	9.654254	H	16.454540	13.266685	15.714398
C	11.782681	6.400010	9.189105	H	17.663771	16.212559	17.355501
C	10.415481	8.837953	9.764912	H	18.435799	16.293486	15.722996
C	9.731818	10.024281	10.001322	H	17.660908	17.757208	16.422531
C	9.801586	12.519816	10.310193	H	13.888177	11.158182	13.423863
C	9.899087	14.974217	10.193823	H	13.090501	11.091566	15.025885
C	8.491786	14.998316	9.936734	H	12.136974	11.570176	13.561525
GO-AA-keto (below)							
C	18.996964	11.109699	10.353297	C	8.389862	15.042497	9.962753
C	18.347008	12.308782	10.551479	C	7.677847	13.848015	9.948274
C	19.095709	13.575672	10.542528	C	8.314389	12.610995	10.157900
C	20.487862	13.574728	10.333457	C	10.278347	6.484588	9.379549
C	21.240900	12.312420	10.305706	C	9.550387	7.691076	9.653543
C	20.459934	11.034835	10.270477	C	8.217878	10.162872	10.060711
C	18.407383	14.828146	10.633751	C	8.166986	7.738338	9.561011
C	21.220982	14.774205	10.144433	C	7.408109	8.943213	9.791798
C	20.546616	16.001413	10.264970	C	7.588712	11.394639	10.061587

C	19.151112	16.051914	10.482879	C	14.563730	6.356507	9.466010
C	21.340820	17.240814	10.249561	C	12.413399	5.267058	9.071120
C	22.710810	17.193817	9.717100	C	13.780914	5.241691	9.052109
C	23.349520	15.975314	9.609901	C	7.551887	16.256783	9.734703
C	22.647133	14.745018	9.877583	C	9.532177	5.248570	8.982297
C	23.322758	13.523806	9.750164	C	16.993828	17.638597	12.390404
C	22.614737	12.310645	9.768592	C	14.102299	13.094238	6.649992
C	16.905247	12.324145	10.701435	C	15.571836	13.379121	6.456109
C	16.234848	13.598867	11.137049	C	16.238388	14.111804	7.626723
C	16.984245	14.868919	10.777488	C	17.325346	15.113648	7.261603
C	16.273016	16.056820	10.691199	C	18.613539	14.561982	6.720776
C	17.001902	17.377937	10.815107	O	26.626869	12.964237	11.232590
C	18.471901	17.315594	10.457574	O	24.697298	13.863598	12.025476
C	20.599895	18.553291	10.212580	O	16.337042	13.647149	12.623993
C	19.130333	18.500969	10.194698	O	21.192383	18.064341	11.452518
C	24.735298	15.928177	9.155275	O	21.220112	22.049196	9.148195
C	25.413599	14.759656	9.116979	O	18.374882	5.802794	7.722772
C	21.300230	19.732157	9.644994	O	19.809397	5.841940	9.473846
C	23.375351	18.426958	9.337110	O	14.273521	7.818779	11.434136
C	22.629223	19.655203	9.323236	O	21.134377	11.471651	11.507328
C	18.424746	19.725145	9.934488	O	14.203785	19.506954	9.421627
C	17.029112	19.692799	9.865595	O	26.616159	17.171028	8.325012
C	16.290512	18.542030	10.149804	O	10.177909	11.240466	12.262590
C	14.847778	16.074358	10.612293	O	6.457296	16.237007	9.188737
C	14.107825	14.892820	10.761727	O	8.077394	17.419270	10.229949
C	14.754750	13.644438	10.828817	O	9.586360	4.723775	7.881482
C	16.150673	11.163048	10.548485	O	8.784530	4.747490	10.004314
C	16.797985	9.906900	10.296063	O	17.970425	17.569880	13.104168
C	18.285761	9.798500	10.491438	O	15.744947	17.922607	12.846294
C	21.066359	9.879043	9.587143	O	6.158314	8.966741	9.760552
C	22.397873	9.938358	9.186105	O	24.947618	9.987003	8.169926
C	23.174078	11.110352	9.290461	O	18.368265	9.405418	11.922288
C	18.915712	8.669288	9.690967	O	12.417284	15.133571	12.435213
C	20.252625	8.766676	9.315869	O	16.187778	13.028175	5.458148
C	24.538685	11.152116	8.766907	O	17.130566	16.314907	7.428413
C	25.304823	12.258221	8.863325	H	26.460449	14.762472	8.800796
C	25.446377	17.192410	8.754217	H	23.141371	20.553183	8.973751
C	24.689440	18.411612	8.899068	H	16.534441	20.610489	9.528358
C	20.521362	20.927448	9.489287	H	22.843620	9.062705	8.712240
C	19.152790	20.915226	9.639743	H	18.587734	21.837051	9.468830
C	14.913473	18.461720	9.931032	H	25.189072	19.339354	8.612653
C	14.153131	17.301277	10.227233	H	26.338097	12.265943	8.511248
C	14.016729	12.460563	10.704173	H	20.720863	7.932330	8.790991
C	14.690485	11.201905	10.566759	H	25.208317	13.822112	12.863307
C	24.824963	13.472724	9.611927	H	15.794772	12.906645	12.965864
C	25.502029	13.381623	11.051129	H	20.603662	22.794870	9.027435
C	18.127592	7.530226	9.399668	H	16.420702	5.495912	8.939759
C	16.097132	8.746099	10.077525	H	12.297330	18.189100	9.635137
C	13.947001	10.036317	10.409532	H	20.137331	5.064716	8.970438
C	12.565970	12.494938	10.638391	H	6.603362	13.880719	9.761010
C	12.614064	14.972973	10.969069	H	14.810820	20.229885	9.179800
C	12.779503	17.293205	10.028162	H	6.507474	11.414378	9.898777
C	16.737129	7.523732	9.638187	H	14.302732	4.351146	8.693129
C	14.645665	8.743552	10.351988	H	11.861070	4.388846	8.737473
C	12.508043	10.050568	10.376459	H	10.551300	10.388253	12.566418

C	11.842855	11.261552	10.533974	H	7.405772	18.107691	10.033669
C	11.878219	13.707367	10.657158	H	8.321078	3.956812	9.649867
C	11.985953	16.163046	10.293655	H	15.826357	18.013191	13.819963
C	10.628994	16.171213	10.022907	H	10.188008	17.099091	9.662307
C	13.850220	7.506380	10.063238	H	7.585705	6.847040	9.324365
C	15.933965	6.382880	9.345243	H	25.877180	10.080125	7.890738
C	18.750881	6.330518	8.759383	H	19.288166	9.564606	12.218182
C	10.455101	13.763480	10.436104	H	13.038061	15.832956	12.726642
C	10.358583	11.279428	10.786198	H	13.719854	12.469164	5.835284
C	11.750899	8.826975	10.104935	H	13.934188	12.604443	7.623327
C	12.393220	7.626865	9.847687	H	13.547359	14.046228	6.685407
C	11.669981	6.447536	9.429117	H	18.392023	13.923134	5.850262
C	10.311942	8.891028	10.001953	H	19.300945	15.373283	6.455524
C	9.633321	10.080130	10.227222	H	19.078279	13.909075	7.478577
C	9.708382	12.586075	10.416452	H	16.679058	13.307244	8.244125
C	9.803650	15.028234	10.172376	H	15.478265	14.621258	8.232363

GO-AA-enol (below)

C	18.967705	11.229963	10.240716	C	8.322764	15.114351	10.043097
C	18.311144	12.424303	10.441190	C	7.617445	13.916035	10.014496
C	19.054075	13.693479	10.442636	C	8.267450	12.678436	10.174908
C	20.450144	13.698697	10.263944	C	10.260386	6.592681	9.175797
C	21.209072	12.439068	10.252061	C	9.528385	7.783549	9.506100
C	20.432266	11.158350	10.184612	C	8.186252	10.233182	10.015892
C	18.358286	14.941454	10.506000	C	8.143150	7.824814	9.441814
C	21.178436	14.901470	10.073966	C	7.380852	9.014737	9.730580
C	20.493475	16.125431	10.162891	C	7.548091	11.459404	10.063123
C	19.095299	16.167837	10.357614	C	14.550341	6.502416	9.182760
C	21.277681	17.371254	10.136014	C	12.402527	5.412517	8.772161
C	22.655602	17.324997	9.624158	C	13.769650	5.402022	8.728374
C	23.308224	16.111181	9.560122	C	7.472775	16.331196	9.885710
C	22.609589	14.880347	9.837117	C	9.519274	5.358312	8.764828
C	23.295822	13.662945	9.740628	C	16.945503	17.711103	12.265974
C	22.594604	12.445462	9.745416	C	14.679296	10.808626	6.862009
C	16.869654	12.431644	10.578424	C	15.751746	11.842383	7.065872
C	16.193371	13.704956	10.996201	C	17.127340	11.503516	6.885769
C	16.933718	14.974199	10.625967	C	18.093515	12.492768	7.002428
C	16.215681	16.156973	10.546956	C	19.551626	12.270646	6.776332
C	16.939234	17.481422	10.685980	O	26.470827	13.003665	11.375320
C	18.407341	17.428106	10.317619	O	24.657082	14.212480	12.013243
C	20.528259	18.676659	10.066248	O	16.304451	13.769918	12.487152
C	19.058033	18.615562	10.045276	O	21.113316	18.217367	11.321798
C	24.704729	16.067375	9.139172	O	21.128811	22.155560	8.936668
C	25.394258	14.904674	9.145172	O	18.397959	6.094959	7.368697
C	21.223509	19.849527	9.480421	O	19.742092	5.958891	9.187662
C	23.314316	18.555799	9.226398	O	14.265720	7.870101	11.221478
C	22.556374	19.776026	9.172107	O	21.079664	11.583202	11.439966
C	18.344589	19.834743	9.779610	O	14.098211	19.629284	9.414292
C	16.947746	19.798857	9.733374	O	26.592981	17.312321	8.327242
C	16.213270	18.649479	10.040730	O	10.176022	11.269463	12.205719
C	14.788238	16.167915	10.497394	O	6.362051	16.327423	9.373134
C	14.058784	14.983796	10.658966	O	8.007496	17.475721	10.412822
C	14.712406	13.739386	10.709743	O	9.580232	4.836344	7.662401
C	16.120144	11.269695	10.426491	O	8.767587	4.848407	9.780238

C	16.771873	10.022009	10.152278	O	17.926161	17.615911	12.971438
C	18.259966	9.914918	10.341749	O	15.703032	17.996719	12.738379
C	21.054396	10.015583	9.493200	O	6.130457	9.026766	9.733891
C	22.396557	10.080854	9.128864	O	24.976097	10.140881	8.190821
C	23.169300	11.250863	9.271132	O	18.344557	9.474743	11.759893
C	18.896782	8.813864	9.508530	O	12.422508	15.190413	12.388439
C	20.242752	8.915458	9.168270	O	15.407349	13.033312	7.371040
C	24.548046	11.300718	8.786091	O	17.749025	13.731713	7.308979
C	25.309114	12.406721	8.914531	H	26.447618	14.910427	8.851002
C	25.411421	17.329554	8.724030	H	23.064741	20.670881	8.809250
C	24.637356	18.543056	8.816163	H	16.447876	20.709675	9.384783
C	20.436607	21.036171	9.301159	H	22.854649	9.213316	8.651693
C	19.068436	21.021496	9.458592	H	18.499916	21.939579	9.277985
C	14.827912	18.571184	9.869044	H	25.133904	19.468559	8.517622
C	14.079178	17.400791	10.159407	H	26.351301	12.417869	8.589554
C	13.980187	12.552481	10.602667	H	20.720192	8.093704	8.630868
C	14.660028	11.299421	10.455149	H	25.131325	14.174143	12.872057
C	24.802361	13.620342	9.644937	H	15.739354	13.050411	12.837090
C	25.419485	13.549597	11.113165	H	20.507891	22.895424	8.804728
C	18.108114	7.692829	9.160448	H	16.407757	5.679564	8.596715
C	16.074921	8.866951	9.898005	H	12.198909	18.293934	9.656496
C	13.921757	10.132298	10.287863	H	20.079506	5.213098	8.644357
C	12.529307	12.579122	10.561625	H	6.537978	13.946139	9.858032
C	12.573456	15.052588	10.911964	H	14.685474	20.390320	9.254800
C	12.698973	17.391684	10.010781	H	6.463503	11.475443	9.924316
C	16.718477	7.670959	9.398679	H	14.292901	4.533329	8.321077
C	14.625557	8.845868	10.180926	H	11.853197	4.543933	8.410498
C	12.482185	10.140044	10.262234	H	10.569570	10.417225	12.482746
C	11.811992	11.343619	10.45166 0	H	7.326511	18.167034	10.265062
C	11.835327	13.786905	10.607756	H	8.309307	4.058680	9.417427
C	11.919713	16.251875	10.280521	H	15.794157	18.066212	13.712860
C	10.554786	16.256481	10.055775	H	10.095570	17.187576	9.727563
C	13.835072	7.617944	9.840693	H	7.562420	6.938318	9.187666
C	15.919422	6.543009	9.049948	H	25.915440	10.235135	7.947219
C	18.733870	6.528343	8.461597	H	19.251909	9.668329	12.073175
C	10.407714	13.838195	10.425127	H	13.093513	15.842923	12.677269
C	10.332295	11.346069	10.726871	H	17.417479	10.482704	6.643903
C	11.728661	8.921651	9.958447	H	16.677046	13.676589	7.397136
C	12.375110	7.737040	9.645350	H	19.797592	11.202830	6.735260
C	11.653821	6.568899	9.193011	H	19.852407	12.743160	5.827718
C	10.287546	8.978398	9.878883	H	20.132723	12.756168	7.573520
C	9.605384	10.155642	10.151444	H	13.786978	11.071001	7.443595
C	9.666960	12.656707	10.400296	H	14.397986	10.790636	5.796332
C	9.742011	15.103937	10.208006	H	15.027723	9.801695	7.130508
GO-CF <sub>3</sub> _DK-keto (below)							
C	18.943634	11.176723	10.262226	C	8.324467	15.102736	9.855055
C	18.294043	12.376174	10.448789	C	7.614089	13.906907	9.844096
C	19.042673	13.642286	10.434619	C	8.255646	12.670217	10.042964
C	20.437254	13.639568	10.247145	C	10.221740	6.535130	9.314870
C	21.188650	12.376503	10.233290	C	9.494016	7.742196	9.589507
C	20.406363	11.099821	10.187962	C	8.161257	10.219710	9.980244
C	18.352417	14.895847	10.488422	C	8.109489	7.786057	9.518429
C	21.172657	14.836862	10.052450	C	7.351738	8.992781	9.745465

C	20.496384	16.065506	10.143027	C	7.530767	11.450822	9.969609
C	19.096842	16.117990	10.333213	C	14.510480	6.432651	9.317272
C	21.289055	17.305296	10.119590	C	12.359350	5.330400	8.960432
C	22.669395	17.251678	9.615726	C	13.726627	5.315514	8.912122
C	23.310320	16.032114	9.539047	C	7.480593	16.321196	9.676951
C	22.602440	14.805534	9.809035	C	9.475739	5.288367	8.954540
C	23.279198	13.582716	9.702953	C	16.898760	17.821613	12.158079
C	22.569576	12.371243	9.715448	C	14.873445	10.612516	6.616828
C	16.850842	12.394114	10.572759	C	15.016821	12.015992	6.103025
C	16.173883	13.677163	10.967028	C	15.790311	13.011576	7.001720
C	16.926430	14.938945	10.591197	C	17.274403	12.742897	7.019062
C	16.215950	16.124849	10.474480	C	18.171556	13.958339	6.624558
C	16.939528	17.446018	10.602442	O	26.523226	12.978535	11.265831
C	18.414766	17.380157	10.268088	O	24.636793	14.021898	11.983266
C	20.545918	18.616985	10.041826	O	16.250837	13.763853	12.456213
C	19.076887	18.561172	9.992935	O	21.112078	18.151630	11.301525
C	24.704519	15.979794	9.112046	O	21.184250	22.093197	8.925846
C	25.382057	14.810453	9.095773	O	18.309153	5.948172	7.502450
C	21.257393	19.785763	9.467115	O	19.742538	5.919357	9.254793
C	23.340969	18.479227	9.229853	O	14.230412	7.876038	11.303178
C	22.593597	19.705811	9.177769	O	21.069090	11.533140	11.432278
C	18.374525	19.778242	9.687966	O	14.139032	19.575912	9.204401
C	16.980593	19.744711	9.598565	O	26.606354	17.211967	8.316208
C	16.233166	18.603947	9.907592	O	10.144035	11.333204	12.140430
C	14.791000	16.139046	10.381981	O	6.374614	16.317337	9.154757
C	14.052208	14.960939	10.547314	O	8.015901	17.466860	10.200731
C	14.699585	13.715103	10.638975	O	9.526433	4.731246	7.869357
C	16.096901	11.231826	10.425203	O	8.734605	4.814043	9.994186
C	16.743717	9.976814	10.175752	O	17.856499	18.181744	12.807342
C	18.229748	9.865211	10.372290	O	15.641529	17.726923	12.664204
C	21.016657	9.948441	9.501299	O	6.101835	9.011141	9.739273
C	22.354961	10.003025	9.122385	O	24.925676	10.037572	8.164634
C	23.134415	11.169700	9.246338	O	18.306030	9.444874	11.797257
C	18.860533	8.749187	9.554180	O	12.393308	15.210835	12.246428
C	20.202127	8.846026	9.198094	O	14.546190	12.408499	5.048388
C	24.508829	11.205979	8.749263	O	17.803164	11.677883	7.282627
C	25.276022	12.309793	8.858685	H	26.433838	14.809787	8.796255
C	25.425356	17.238655	8.713244	H	23.111717	20.598467	8.823286
C	24.664347	18.459000	8.821210	H	16.493385	20.651020	9.221541
C	20.479736	20.975351	9.267798	H	22.802998	9.128514	8.648630
C	19.107620	20.961731	9.380924	H	18.545341	21.878590	9.177315
C	14.852349	18.526756	9.704552	H	25.169416	19.383072	8.532547
C	14.092161	17.366610	10.005065	H	26.315989	12.313770	8.527084
C	13.961395	12.528646	10.542032	H	20.673088	8.019381	8.664151
C	14.636453	11.268770	10.434298	H	25.130466	13.988205	12.831563
C	24.783281	13.528490	9.590182	H	15.712665	13.024367	12.806769
C	25.428520	13.452787	11.045507	H	20.568899	22.834574	8.776407
C	18.070520	7.620456	9.233297	H	16.364180	5.587402	8.754576
C	16.042721	8.818702	9.944724	H	12.226552	18.257858	9.446995
C	13.892903	10.101328	10.287645	H	20.066114	5.157669	8.725447
C	12.511655	12.561730	10.478655	H	6.536071	13.939097	9.678018
C	12.563374	15.042556	10.776838	H	14.735239	20.326321	9.028768
C	12.714922	17.360630	9.829470	H	6.447496	11.467285	9.820976
C	16.681259	7.606629	9.479531	H	14.247226	4.429739	8.539763
C	14.593199	8.810201	10.226459	H	11.806824	4.448598	8.637221

C	12.454418	10.115007	10.253403	H	10.514114	10.482667	12.453135
C	11.789322	11.327670	10.397481	H	7.339495	18.160460	10.042597
C	11.823751	13.774255	10.486523	H	8.273238	4.011681	9.664322
C	11.924339	16.231125	10.109966	H	15.708765	17.980391	13.609630
C	10.562530	16.236824	9.865439	H	10.111764	17.162722	9.511217
C	13.799055	7.573905	9.932539	H	7.525994	6.890985	9.303077
C	15.878867	6.467676	9.176497	H	25.859873	10.127904	7.900679
C	18.688131	6.438496	8.556122	H	19.224243	9.600123	12.100159
C	10.398739	13.827815	10.284416	H	13.089294	15.835343	12.538568
C	10.308028	11.348303	10.661495	H	14.419037	9.970078	5.854661
C	11.697029	8.889168	9.996127	H	15.850500	10.220395	6.939206
C	12.339252	7.690327	9.734070	H	14.236882	10.630341	7.517606
C	11.614540	6.505857	9.332912	H	15.434185	12.891660	8.039888
C	10.256613	8.949123	9.911669	H	15.572063	14.030856	6.662678
C	9.578806	10.140032	10.129657	F	17.798920	15.082873	7.309096
C	9.652610	12.649499	10.282602	F	19.476639	13.732742	6.875792
C	9.742134	15.091125	10.032586	F	18.023857	14.219093	5.294004

GO-CF<sub>3</sub>\_DK-enol (below)

C	18.966658	11.158887	10.273727	C	8.347167	15.068928	9.919359
C	18.316404	12.357465	10.460569	C	7.637296	13.873261	9.925667
C	19.066654	13.623011	10.447489	C	8.280293	12.639340	10.135761
C	20.462437	13.620190	10.271450	C	10.247263	6.493040	9.468182
C	21.212734	12.355849	10.250731	C	9.520617	7.707346	9.712741
C	20.429077	11.082257	10.195028	C	8.188190	10.189532	10.067458
C	18.375999	14.875238	10.495225	C	8.137309	7.753061	9.622044
C	21.197706	14.817722	10.077554	C	7.379397	8.964645	9.817286
C	20.519590	16.046307	10.160189	C	7.556601	11.419665	10.059081
C	19.119820	16.097530	10.341529	C	14.535224	6.394757	9.453860
C	21.310221	17.287842	10.135480	C	12.384306	5.281525	9.136213
C	22.690815	17.233160	9.632236	C	13.751163	5.267921	9.078413
C	23.333057	16.013660	9.559918	C	7.503026	16.282055	9.711232
C	22.627100	14.786378	9.833067	C	9.499416	5.235051	9.152150
C	23.303064	13.562964	9.720820	C	16.931807	17.689705	12.187772
C	22.591480	12.352408	9.727497	C	14.141044	12.694197	7.207894
C	16.875025	12.372158	10.606625	C	15.551979	12.200413	7.127260
C	16.203506	13.657072	10.999168	C	16.652767	13.114984	7.043883
C	16.950874	14.914858	10.602224	C	17.910717	12.578626	6.858249
C	16.237452	16.099287	10.486151	C	19.139353	13.455857	6.627046
C	16.961445	17.423473	10.613561	O	26.594429	12.999846	11.235859
C	18.437155	17.359118	10.278313	O	24.647251	13.872145	12.015710
C	20.566656	18.597525	10.053242	O	16.307768	13.757499	12.486355
C	19.097227	18.541880	10.006878	O	21.133192	18.137978	11.316027
C	24.727018	15.961772	9.131207	O	21.199795	22.073170	8.933614
C	25.404682	14.792667	9.112002	O	18.275486	5.928533	7.544318
C	21.275627	19.765965	9.475556	O	19.764383	5.901192	9.250299
C	23.360325	18.459925	9.240883	O	14.267646	7.864817	11.421293
C	22.611311	19.685888	9.184298	O	21.094439	11.502996	11.443563
C	18.392227	19.759991	9.713619	O	14.157945	19.545172	9.218676
C	16.997124	19.725624	9.629370	O	26.626728	17.194599	8.329467
C	16.253181	18.579727	9.928893	O	10.162574	11.304695	12.240015
C	14.812433	16.113668	10.412016	O	6.401414	16.264612	9.179822
C	14.075428	14.936265	10.599028	O	8.032057	17.440323	10.213526
C	14.723787	13.691861	10.700755	O	9.552986	4.630670	8.092465



C	16.122305	11.207722	10.487743	O	8.751367	4.806740	10.207285
C	16.768696	9.951784	10.241898	O	17.898626	17.622129	12.914577
C	18.259190	9.845980	10.408312	O	15.676954	17.974859	12.627381
C	21.032145	9.933239	9.498412	O	6.130119	8.989432	9.772204
C	22.367630	9.989870	9.110706	O	24.936682	10.025743	8.149479
C	23.150053	11.153927	9.243313	O	18.371025	9.437740	11.833683
C	18.878996	8.728821	9.582438	O	12.421028	15.213246	12.301727
C	20.214270	8.830442	9.203136	O	15.768383	10.942255	7.089675
C	24.522732	11.191192	8.741870	O	18.137142	11.292718	6.803271
C	25.292610	12.292897	8.855199	H	26.456558	14.792934	8.812966
C	25.446487	17.220942	8.728820	H	23.129126	20.577785	8.827425
C	24.683861	18.440596	8.832945	H	16.507412	20.635538	9.264199
C	20.496553	20.955956	9.281274	H	22.811953	9.119331	8.626348
C	19.125437	20.944593	9.406615	H	18.563393	21.863081	9.209498
C	14.873258	18.498281	9.720987	H	25.187637	19.364285	8.541029
C	14.113413	17.338284	10.026314	H	26.332184	12.296629	8.522259
C	13.986325	12.503191	10.631132	H	20.678856	8.005047	8.661869
C	14.661999	11.243917	10.519738	H	25.148851	13.824308	12.858955
C	24.806419	13.507699	9.599464	H	15.744186	13.045094	12.852736
C	25.467997	13.409145	11.045399	H	20.584412	22.815752	8.790432
C	18.085451	7.596907	9.283066	H	16.382795	5.546286	8.877781
C	16.067257	8.791479	10.030575	H	12.244548	18.221024	9.464748
C	13.919490	10.075743	10.383325	H	20.074257	5.142958	8.708096
C	12.536420	12.535753	10.574145	H	6.559567	13.902426	9.757901
C	12.587416	15.021921	10.835075	H	14.753262	20.296711	9.044508
C	12.735802	17.328083	9.853924	H	6.474030	11.435089	9.904667
C	16.702477	7.578954	9.563726	H	14.270532	4.376417	8.718107
C	14.620718	8.784780	10.326699	H	11.830930	4.393195	8.833549
C	12.480684	10.087631	10.357784	H	10.541231	10.458283	12.553526
C	11.814238	11.300288	10.499186	H	7.355178	18.128645	10.035425
C	11.847775	13.748881	10.566459	H	8.289884	3.992370	9.908429
C	11.946959	16.200499	10.150556	H	15.747292	18.069584	13.601473
C	10.584196	16.202694	9.910850	H	10.132115	17.123650	9.545280
C	13.827024	7.544670	10.057119	H	7.555193	6.856694	9.408225
C	15.900979	6.432003	9.292282	H	25.869267	10.117857	7.880375
C	18.686197	6.418024	8.586370	H	19.295204	9.600193	12.114395
C	10.422825	13.799593	10.365973	H	13.053012	15.913460	12.566022
C	10.332371	11.320590	10.761068	H	13.497643	11.932126	7.663879
C	11.723581	8.858353	10.112332	H	16.501516	14.189737	7.097334
C	12.365708	7.656335	9.864970	H	14.070904	13.636094	7.768457
C	11.640361	6.464159	9.486416	H	13.775732	12.883379	6.184689
C	10.283031	8.917622	10.023546	H	17.102924	10.880057	6.931993
C	9.604842	10.110569	10.228323	F	18.966990	14.708307	7.136988
C	9.676895	12.620481	10.376736	F	20.252745	12.924119	7.192921
C	9.765034	15.059685	10.096888	F	19.383007	13.589525	5.291326

GO-MAA-keto (below)

C	18.952488	11.139504	10.190342	C	7.628166	13.852086	9.746121
C	18.299301	12.339825	10.370480	C	8.267865	12.617762	9.961530
C	19.046249	13.607562	10.360875	C	10.243303	6.477604	9.272208
C	20.441389	13.605649	10.172085	C	9.514108	7.690765	9.514579
C	21.196560	12.344085	10.174365	C	8.177458	10.168982	9.875663
C	20.416817	11.064329	10.135717	C	8.131675	7.736612	9.409956
C	18.353540	14.858896	10.419237	C	7.371549	8.946048	9.609674

C	21.172478	14.803300	9.965220	C	7.545523	11.399309	9.867110
C	20.492525	16.031048	10.049627	C	14.531792	6.374592	9.310708
C	19.094980	16.081524	10.254601	C	12.383390	5.265129	8.964146
C	21.283054	17.272627	10.009500	C	13.750827	5.248744	8.924910
C	22.655861	17.216675	9.484632	C	7.494617	16.260412	9.530241
C	23.301588	15.998949	9.420934	C	9.498679	5.221011	8.942133
C	22.601734	14.773722	9.716952	C	16.939224	17.702145	12.141849
C	23.283962	13.552796	9.631666	C	12.922905	12.910345	6.889498
C	22.580416	12.337277	9.663554	C	14.177453	12.766549	6.076488
C	16.856049	12.356179	10.499267	C	15.518225	12.971041	6.795790
C	16.182325	13.633174	10.916776	C	15.819138	14.439340	7.058187
C	16.928493	14.899402	10.545137	C	18.201504	13.877479	6.952693
C	16.215727	16.083761	10.450405	O	26.523182	12.999976	11.220317
C	16.942783	17.405933	10.571123	O	24.630140	14.053415	11.903630
C	18.411583	17.343653	10.206879	O	16.285378	13.695157	12.405854
C	20.538719	18.581320	9.939535	O	21.129932	18.124088	11.192320
C	19.068134	18.525774	9.924522	O	21.148594	22.046221	8.767791
C	24.691986	15.944887	8.982128	O	18.342464	5.866761	7.516799
C	25.378204	14.780458	8.995483	O	19.765211	5.866125	9.278170
C	21.236067	19.746622	9.340139	O	14.245811	7.851377	11.268644
C	23.317123	18.441086	9.071695	O	21.066669	11.513578	11.380493
C	22.565500	19.664686	9.019727	O	14.128831	19.532093	9.202816
C	18.360580	19.746189	9.648769	O	26.569862	17.169041	8.119296
C	16.964500	19.714050	9.595860	O	10.129448	11.261871	12.080474
C	16.226078	18.567316	9.901337	O	6.396070	16.235474	8.992594
C	14.789747	16.097975	10.378710	O	8.020413	17.425783	10.017885
C	14.053797	14.918253	10.543281	O	9.560810	4.625169	7.878221
C	14.702825	13.672524	10.614265	O	8.743958	4.785011	9.989012
C	16.104445	11.192539	10.355611	O	17.932978	17.797445	12.829010
C	16.754999	9.936316	10.114105	O	15.674815	17.829657	12.624109
C	18.240547	9.828588	10.322646	O	6.122609	8.970290	9.558101
C	21.035778	9.904080	9.471501	O	24.957136	9.988723	8.167442
C	22.377901	9.958017	9.105380	O	18.308386	9.434309	11.754234
C	23.152279	11.130330	9.217144	O	12.378011	15.169373	12.228841
C	18.878960	8.700244	9.526933	O	14.179963	12.475411	4.887759
C	20.223839	8.795363	9.178691	O	14.964221	15.290576	7.226624
C	24.529961	11.165354	8.728166	O	17.126719	14.821458	7.132348
C	25.290785	12.275225	8.820395	H	26.428368	14.778417	8.690588
C	25.397760	17.198868	8.541752	H	23.074089	20.554724	8.645622
C	24.633944	18.418127	8.641731	H	16.467506	20.626143	9.246826
C	20.454376	20.935261	9.153089	H	22.834494	9.077997	8.650226
C	19.087387	20.927883	9.319133	H	18.520988	21.845667	9.131168
C	14.845863	18.485970	9.698950	H	25.131054	19.338970	8.329858
C	14.091166	17.322517	9.998345	H	26.332205	12.277588	8.493161
C	13.967220	12.485242	10.511445	H	20.700686	7.960068	8.663175
C	14.643969	11.228071	10.377055	H	25.118958	14.040344	12.755280
C	24.789043	13.506564	9.524214	H	15.727426	12.969210	12.753738
C	25.428558	13.466328	10.982939	H	20.529793	22.787142	8.630621
C	18.091356	7.564688	9.221128	H	16.388971	5.519782	8.773925
C	16.056978	8.773911	9.897214	H	12.230609	18.203274	9.411493
C	13.903725	10.059216	10.228029	H	20.093063	5.096651	8.762872
C	12.516460	12.515085	10.457368	H	6.554046	13.881199	9.556617
C	12.562521	14.996088	10.762157	H	14.728448	20.265913	8.975964
C	12.717356	17.311123	9.807306	H	6.465112	11.415751	9.698845
C	16.700592	7.553657	9.459259	H	14.273079	4.355671	8.572911

C	14.606575	8.768537	10.175595	H	11.832660	4.377592	8.654070
C	12.465065	10.068929	10.200607	H	10.504182	10.412142	12.389441
C	11.797135	11.279202	10.356377	H	7.345144	18.111609	9.824843
C	11.826761	13.726249	10.467388	H	8.284814	3.972451	9.681788
C	11.928920	16.179785	10.081878	H	15.765272	17.975924	13.590077
C	10.572557	16.182827	9.811941	H	10.129055	17.106480	9.443666
C	13.816188	7.526599	9.902145	H	7.552007	6.841654	9.184069
C	15.900809	6.408131	9.175318	H	25.894468	10.077523	7.913972
C	18.713984	6.372821	8.565717	H	19.225397	9.591733	12.059568
C	10.404520	13.777075	10.241636	H	13.024991	15.847576	12.513767
C	10.312621	11.294321	10.604482	H	12.039203	12.840910	6.245423
C	11.711842	8.839943	9.941771	H	12.888557	12.112791	7.650428
C	12.357122	7.638837	9.695781	H	12.939306	13.867105	7.433118
C	11.636080	6.448087	9.306990	H	16.294254	12.497176	6.182219
C	10.272785	8.898719	9.841355	H	15.504520	12.468662	7.780000
C	9.591876	10.089683	10.050674	H	18.099146	13.010614	7.621389
C	9.660837	12.597458	10.225641	H	18.262783	13.546474	5.905196
C	9.750206	15.038158	9.968550	H	19.113108	14.426872	7.216146
C	8.336842	15.048562	9.758066				

GO-MAA-enol (below)

C	18.887667	11.133153	10.244670	C	7.544085	13.842443	10.048660
C	18.234711	12.329309	10.434180	C	8.193236	12.605038	10.216123
C	18.982368	13.595994	10.437765	C	10.169028	6.509521	9.253564
C	20.379507	13.596430	10.269522	C	9.440837	7.704229	9.575694
C	21.131859	12.333241	10.258425	C	8.105601	10.159265	10.068240
C	20.351097	11.058145	10.190806	C	8.055943	7.747220	9.510636
C	18.290773	14.846854	10.502930	C	7.296621	8.942666	9.783050
C	21.114971	14.796567	10.089785	C	7.470934	11.386752	10.111250
C	20.433346	16.024067	10.170297	C	14.457960	6.398703	9.272749
C	19.033030	16.070871	10.353302	C	12.305669	5.313980	8.872328
C	21.218428	17.268719	10.122414	C	13.673371	5.295219	8.833793
C	22.598633	17.210896	9.617079	C	7.401882	16.255602	9.900368
C	23.248451	15.994093	9.570486	C	9.421653	5.281343	8.834425
C	22.545942	14.767715	9.855508	C	16.880213	17.661446	12.217297
C	23.227240	13.545872	9.761526	C	13.499602	12.664233	7.194814
C	22.520172	12.332609	9.761276	C	14.984337	12.788651	7.159641
C	16.793873	12.341550	10.575680	C	15.657404	13.983960	7.252325
C	16.125193	13.616503	11.002116	C	17.088259	14.005342	7.114821
C	16.865561	14.883730	10.622713	C	19.054842	15.312483	6.925916
C	16.149548	16.066969	10.532942	O	26.444662	12.962619	11.382568
C	16.875921	17.392641	10.643965	O	24.555252	14.031120	12.050544
C	18.345003	17.329201	10.281948	O	16.250263	13.681467	12.490227
C	20.466599	18.572544	10.009475	O	21.041666	18.147711	11.280700
C	18.996971	18.508955	9.978854	O	21.068455	22.009504	8.753918
C	24.645464	15.942061	9.151185	O	18.261982	5.880641	7.512432
C	25.330818	14.777151	9.164092	O	19.709785	5.885864	9.252565
C	21.164791	19.727892	9.393322	O	14.185848	7.805411	11.283202
C	23.260490	18.432625	9.197411	O	20.994514	11.481534	11.450490
C	22.501635	19.649376	9.103796	O	14.030882	19.532755	9.375874
C	18.284321	19.717976	9.668076	O	26.540304	17.169682	8.330747
C	16.887577	19.681267	9.621389	O	10.095744	11.204863	12.255054
C	16.151520	18.546276	9.971484	O	6.289641	16.247341	9.391080
C	14.722127	16.080400	10.488447	O	7.939571	17.405010	10.413557

C	13.989469	14.900482	10.670967	O	9.468048	4.779543	7.722344
C	14.640985	13.654767	10.729536	O	8.681016	4.756396	9.849905
C	16.041332	11.180531	10.434021	O	17.859816	17.578224	12.925617
C	16.689653	9.929133	10.168843	O	15.639342	17.967777	12.681135
C	18.176989	9.820670	10.361262	O	6.046418	8.962347	9.770230
C	20.969742	9.908356	9.509333	O	24.897650	10.015093	8.220167
C	22.313354	9.967077	9.147943	O	18.258167	9.406996	11.788332
C	23.090689	11.133953	9.290888	O	12.362921	15.137009	12.407080
C	18.813282	8.703285	9.548496	O	15.625375	11.627290	6.997451
C	20.157709	8.804332	9.199820	O	17.800699	12.984149	6.971589
C	24.472691	11.175837	8.814808	O	17.628798	15.250758	7.140241
C	25.239862	12.277247	8.950045	H	26.385025	14.777348	8.872869
C	25.357697	17.197117	8.723701	H	23.011883	20.533978	8.719050
C	24.585745	18.412710	8.793995	H	16.389528	20.577408	9.234388
C	20.376793	20.904100	9.159356	H	22.770176	9.095891	8.676430
C	19.007725	20.892397	9.306319	H	18.438866	21.801283	9.085373
C	14.763065	18.474169	9.825612	H	25.083242	19.332527	8.479815
C	14.013966	17.310371	10.138224	H	26.285343	12.282008	8.635772
C	13.904719	12.467733	10.638226	H	20.634344	7.977888	8.670591
C	14.581828	11.213927	10.478454	H	25.036085	14.008635	12.906489
C	24.733513	13.497542	9.669727	H	15.715052	12.942191	12.845657
C	25.357016	13.440078	11.135087	H	20.446440	22.742022	8.589397
C	18.024218	7.573790	9.224862	H	16.311342	5.555295	8.706966
C	15.990967	8.771765	9.933387	H	12.132692	18.203144	9.638674
C	13.840890	10.048014	10.318471	H	20.034363	5.121113	8.728484
C	12.453537	12.498550	10.608063	H	6.464446	13.872857	9.894032
C	12.505315	14.976828	10.933012	H	14.616043	20.297539	9.227000
C	12.632668	17.303181	9.999331	H	6.386227	11.404559	9.973043
C	16.632057	7.562717	9.462046	H	14.193268	4.418213	8.440602
C	14.542644	8.759807	10.221104	H	11.752748	4.443385	8.520372
C	12.401418	10.058455	10.308573	H	10.487603	10.353900	12.538519
C	11.733700	11.263866	10.500854	H	7.258762	18.095671	10.261658
C	11.762748	13.709818	10.645028	H	8.217818	3.972556	9.480343
C	11.851950	16.168678	10.286133	H	15.730405	18.061794	13.653623
C	10.485841	16.175343	10.065346	H	10.029180	17.104692	9.728239
C	13.747319	7.528105	9.910153	H	7.473868	6.859605	9.263009
C	15.827683	6.430060	9.141554	H	25.835464	10.108644	7.970640
C	18.645010	6.388884	8.556450	H	19.169346	9.592502	12.095768
C	10.335798	13.762361	10.459799	H	13.020386	15.809592	12.680348
C	10.254146	11.271230	10.776620	H	13.202038	11.857762	7.879762
C	11.644617	8.838813	10.018735	H	15.113813	14.915603	7.386978
C	12.286963	7.648806	9.718654	H	13.024115	13.601299	7.507832
C	11.561763	6.478728	9.277172	H	13.130557	12.390820	6.193521
C	10.203625	8.899374	9.940877	H	16.616020	11.868690	6.960145
C	9.524673	10.079623	10.206317	H	19.584841	14.657814	7.629947
C	9.592331	12.581598	10.441141	H	19.299971	15.007939	5.898479
C	9.670902	15.027409	10.231219	H	19.327198	16.360365	7.093393
C	8.251061	15.039353	10.067134				
GO-DMM-keto (below)							
C	18.983673	11.113899	10.292541	C	7.654380	13.817480	9.867412
C	18.329723	12.314379	10.453397	C	8.295623	12.586021	10.093264
C	19.076683	13.581357	10.431775	C	10.274055	6.460427	9.360334
C	20.471806	13.578873	10.248034	C	9.542881	7.666430	9.631413

C	21.225330	12.316044	10.250379	C	8.204723	10.137721	10.030376
C	20.447020	11.038740	10.226830	C	8.159088	7.710209	9.544384
C	18.387980	14.833776	10.495263	C	7.397846	8.913267	9.775121
C	21.207907	14.775990	10.053120	C	7.571513	11.366407	10.020055
C	20.531080	16.005213	10.141660	C	14.562358	6.342755	9.456299
C	19.131605	16.056499	10.338717	C	12.414681	5.250175	9.052497
C	21.321136	17.246653	10.101523	C	13.782503	5.227032	9.040347
C	22.699856	17.188288	9.592659	C	7.515491	16.221458	9.618696
C	23.343931	15.969065	9.530472	C	9.532783	5.216029	8.980751
C	22.638342	14.743020	9.809538	C	16.950871	17.701654	12.179317
C	23.314816	13.519566	9.708203	C	14.003769	13.527122	6.623147
C	22.605350	12.307178	9.730218	C	14.738345	14.831396	6.866813
C	16.888857	12.327547	10.590620	C	16.222956	14.619029	7.073808
C	16.214422	13.609972	10.982756	C	18.372957	15.505026	6.633828
C	16.962984	14.874011	10.608980	C	12.024117	12.323150	7.095850
C	16.250414	16.057493	10.498875	O	26.602306	12.973098	11.236645
C	16.973700	17.382847	10.615077	O	24.657345	13.863024	12.001920
C	18.447460	17.318216	10.269745	O	16.309004	13.693488	12.473592
C	20.574850	18.555490	10.007439	O	21.150829	18.112022	11.271020
C	19.104980	18.497501	9.975037	O	21.192472	22.001698	8.782434
C	24.739281	15.915742	9.105513	O	18.427814	5.738023	7.797866
C	25.417234	14.746398	9.094326	O	19.792749	5.821673	9.604439
C	21.278027	19.714508	9.403121	O	14.260418	7.824374	11.408242
C	23.366894	18.411957	9.187782	O	21.107864	11.494411	11.466238
C	22.613745	19.633451	9.110725	O	14.165475	19.495159	9.207469
C	18.398018	19.711214	9.668034	O	26.643478	17.147984	8.312045
C	17.002811	19.675909	9.600288	O	10.160683	11.249704	12.213694
C	16.261496	18.534336	9.920938	O	6.388665	16.182941	9.143503
C	14.823943	16.068581	10.418416	O	8.069631	17.404070	10.027617
C	14.087279	14.889568	10.592366	O	9.603734	4.660288	7.895719
C	14.735346	13.644782	10.680563	O	8.768264	4.740769	10.003254
C	16.136715	11.164708	10.466272	O	17.936504	17.821541	12.874036
C	16.786066	9.904968	10.247823	O	15.679955	17.820242	12.647268
C	18.273048	9.805367	10.452791	O	6.147794	8.932547	9.753718
C	21.060543	9.870623	9.570312	O	24.952887	9.967776	8.176872
C	22.394531	9.926501	9.176735	O	18.347898	9.443853	11.893754
C	23.168434	11.101234	9.270953	O	12.416471	15.182492	12.275795
C	18.911972	8.658491	9.687115	O	14.380841	12.641044	5.878481
C	20.251356	8.749256	9.320225	O	16.720474	13.724089	7.735127
C	24.538500	11.137418	8.761271	O	16.938906	15.594685	6.458961
C	25.305437	12.243127	8.857930	O	12.835501	13.502025	7.313921
C	25.458935	17.173857	8.698803	H	26.470057	14.745621	8.798326
C	24.691675	18.391678	8.783317	H	23.127239	20.520288	8.735457
C	20.495499	20.896524	9.179599	H	16.510160	20.578720	9.221838
C	19.126406	20.888227	9.324009	H	22.845663	9.044296	8.720475
C	14.881847	18.450905	9.715221	H	18.560619	21.800537	9.109568
C	14.125051	17.289639	10.018435	H	25.193403	19.313576	8.481986
C	13.998416	12.457891	10.597838	H	26.342781	12.246535	8.517890
C	14.676490	11.200147	10.484213	H	20.724665	7.903850	8.817415
C	24.818645	13.464856	9.590818	H	25.158453	13.825837	12.845965
C	25.477379	13.383097	11.039114	H	15.819184	12.921716	12.825485
C	18.127892	7.511680	9.418668	H	20.574305	22.739416	8.626947
C	16.088810	8.739333	10.049335	H	16.424313	5.476586	8.953984
C	13.935646	10.030086	10.356646	H	12.262589	18.159557	9.416821
C	12.547860	12.486675	10.557060	H	20.137955	5.028747	9.138614

C	12.597176	14.972850	10.812185	H	6.577446	13.844704	9.694396
C	12.751044	17.271643	9.820317	H	14.759106	20.248207	9.034509
C	16.734482	7.510567	9.637654	H	6.489302	11.381530	9.863632
C	14.636624	8.738494	10.317818	H	14.306809	4.335829	8.686627
C	12.495817	10.039868	10.333714	H	11.865999	4.369984	8.718552
C	11.827593	11.250234	10.483037	H	10.561261	10.415787	12.533003
C	11.858604	13.698242	10.550409	H	7.384485	18.082745	9.844549
C	11.962728	16.143570	10.111881	H	8.310988	3.941506	9.660428
C	10.604868	16.143108	9.849967	H	15.759117	17.984541	13.611197
C	13.843799	7.496415	10.039776	H	10.160072	17.059654	9.466354
C	15.934177	6.366678	9.348811	H	7.578683	6.816702	9.315211
C	18.766005	6.292881	8.833340	H	25.885616	10.058553	7.907628
C	10.435724	13.747580	10.335272	H	19.264551	9.617962	12.191266
C	10.344228	11.268206	10.737496	H	13.140384	15.776036	12.564039
C	11.741867	8.812237	10.071796	H	14.333974	15.336068	7.756886
C	12.386926	7.612510	9.819480	H	14.567863	15.492431	6.004472
C	11.666519	6.429257	9.405319	H	18.638256	15.630478	7.691999
C	10.302045	8.871668	9.970891	H	18.738964	14.530747	6.282845
C	9.621683	10.060447	10.191631	H	18.790291	16.319511	6.032517
C	9.690521	12.567637	10.345779	H	11.778181	12.220915	6.030354
C	9.780663	15.004692	10.040203	H	12.561579	11.425653	7.431216
C	8.363951	15.013935	9.848432	H	11.120352	12.478558	7.694328

GO-DMM-enol (below)

C	18.967607	11.171733	10.164816	C	7.636304	13.878268	9.896338
C	18.316399	12.369448	10.352730	C	8.280383	12.643371	10.098135
C	19.065784	13.634648	10.360989	C	10.248740	6.517200	9.325926
C	20.462416	13.632292	10.191706	C	9.521391	7.722360	9.608385
C	21.212395	12.367412	10.174496	C	8.188419	10.194204	10.020896
C	20.430519	11.093743	10.108356	C	8.136398	7.764989	9.540756
C	18.377180	14.886555	10.437011	C	7.378440	8.969682	9.773811
C	21.200693	14.831667	10.021809	C	7.555995	11.424290	10.023070
C	20.523266	16.060339	10.118799	C	14.537963	6.414326	9.303577
C	19.122612	16.110123	10.303089	C	12.384235	5.312350	8.963266
C	21.312634	17.302256	10.083638	C	13.751232	5.295981	8.907869
C	22.692238	17.245584	9.576306	C	7.500108	16.288256	9.697639
C	23.337336	16.027035	9.511036	C	9.500359	5.273594	8.959238
C	22.631367	14.799908	9.783055	C	16.943855	17.733583	12.152752
C	23.308649	13.576831	9.674970	C	14.894434	13.514279	7.115452
C	22.598976	12.364891	9.672898	C	15.601888	14.705647	7.188326
C	16.876003	12.383459	10.493912	C	17.013102	14.620839	7.066822
C	16.206808	13.658716	10.918028	C	19.092875	15.742473	6.868755
C	16.951546	14.925858	10.550118	C	12.865376	12.273538	7.042201
C	16.238152	16.109945	10.460291	O	26.547874	12.985637	11.256763
C	16.963112	17.432817	10.583412	O	24.655924	14.026244	11.962775
C	18.437023	17.370260	10.239019	O	16.321524	13.719387	12.408478
C	20.563847	18.610319	9.985674	O	21.137873	18.168503	11.250904
C	19.094154	18.550161	9.948565	O	21.179377	22.056568	8.760954
C	24.732592	15.975439	9.085939	O	18.336540	5.873119	7.507605
C	25.412069	14.807123	9.075411	O	19.786161	5.916585	9.245836
C	21.267174	19.769539	9.382553	O	14.280181	7.869266	11.281359
C	23.358805	18.470118	9.172673	O	21.077822	11.514795	11.367252
C	22.604298	19.690483	9.094624	O	14.148279	19.554243	9.206022
C	18.385799	19.762331	9.638862	O	26.635101	17.207045	8.290649

C	16.990181	19.727209	9.573125	O	10.174221	11.292192	12.184952
C	16.248774	18.587805	9.898837	O	6.395892	16.273804	9.171572
C	14.811762	16.122906	10.393109	O	8.030672	17.442804	10.206380
C	14.076421	14.944216	10.564786	O	9.539734	4.730018	7.866714
C	14.725134	13.698781	10.632983	O	8.769544	4.786381	10.000193
C	16.123146	11.221983	10.356840	O	17.931299	17.834030	12.848197
C	16.769958	9.967937	10.103646	O	15.675155	17.856438	12.625685
C	18.257542	9.860422	10.291902	O	6.128236	8.990183	9.760798
C	21.044466	9.941703	9.425753	O	24.974585	10.033195	8.148174
C	22.386454	9.998775	9.060085	O	18.343594	9.455388	11.720914
C	23.165846	11.164721	9.201701	O	12.422619	15.206684	12.268646
C	18.889343	8.736229	9.485872	O	15.483962	12.346472	6.965371
C	20.230558	8.836130	9.125508	O	17.646990	13.531346	6.926232
C	24.547684	11.201619	8.726054	O	17.671337	15.805596	7.107963
C	25.313774	12.305205	8.847163	O	13.561062	13.532265	7.196477
C	25.451233	17.233545	8.679838	H	26.464632	14.807366	8.778501
C	24.683926	18.450779	8.768119	H	23.117195	20.578102	8.720534
C	20.483273	20.949635	9.155074	H	16.497643	20.629501	9.193172
C	19.113384	20.938961	9.293467	H	22.840771	9.126426	8.588264
C	14.866678	18.507563	9.704384	H	18.547131	21.849951	9.074549
C	14.110180	17.346798	10.011292	H	25.184866	19.373396	8.467866
C	13.988076	12.512081	10.542213	H	26.358704	12.307684	8.531147
C	14.663942	11.256092	10.400206	H	20.704037	8.006863	8.597633
C	24.813705	13.525074	9.571674	H	25.147018	13.997077	12.812716
C	25.452656	13.456049	11.030010	H	15.801242	12.965976	12.756401
C	18.099630	7.600158	9.187004	H	20.559681	22.791782	8.599783
C	16.070574	8.806249	9.890903	H	16.387552	5.563748	8.734107
C	13.922365	10.087280	10.265331	H	12.241680	18.228361	9.445878
C	12.537573	12.541636	10.511255	H	20.111357	5.140995	8.738299
C	12.588533	15.024147	10.799565	H	6.557781	13.908119	9.733983
C	12.732758	17.335182	9.834490	H	14.742595	20.305016	9.025635
C	16.710150	7.589671	9.437781	H	6.472116	11.440116	9.878579
C	14.625051	8.797992	10.192224	H	14.268996	4.408798	8.535071
C	12.482754	10.096390	10.264938	H	11.829574	4.430121	8.644692
C	11.816398	11.305628	10.432278	H	10.561610	10.446813	12.490271
C	11.848584	13.753183	10.524172	H	7.353043	18.132303	10.035968
C	11.945731	16.206274	10.125312	H	8.304260	3.988548	9.664714
C	10.582693	16.208973	9.886200	H	15.759095	18.006130	13.591641
C	13.830435	7.558294	9.919027	H	10.130021	17.131828	9.526274
C	15.905694	6.447329	9.152862	H	7.553613	6.870522	9.320569
C	18.719954	6.403132	8.540587	H	25.913645	10.123332	7.901734
C	10.423381	13.803453	10.328532	H	19.254879	9.645638	12.025014
C	10.336576	11.321483	10.705679	H	13.111290	15.844108	12.549698
C	11.725939	8.869273	10.009271	H	15.091079	15.655653	7.303792
C	12.368164	7.672122	9.737474	H	16.519817	12.608294	6.923409
C	11.641610	6.488055	9.338947	H	19.572975	15.010954	7.531388
C	10.284786	8.927573	9.935009	H	19.291775	15.467039	5.823025
C	9.606766	10.116209	10.165379	H	19.464647	16.752295	7.076335
C	9.678246	12.623684	10.333200	H	12.983788	11.895914	6.016970
C	9.764206	15.064879	10.067341	H	13.239561	11.528395	7.755694
C	8.345826	15.074183	9.893501	H	11.815268	12.504824	7.249181

Spectroscopic results of keto-enol tautomerism of Acetylacetone (AA), Methyl acetoacetate (MAA), and Dimethyl malonate (DMM) in the presence of G, GO, and PGc

Similar to 1,1,1 trifluoromethyl 2,5-pentanedione (CF<sub>3</sub>\_DK), the characteristic band in the UV-vis spectrum near 255-275 nm was responsible for the  $\pi \rightarrow \pi^*$  transition of the enol form containing a pseudo-aromatic structure with an intramolecular H-bonding.<sup>4</sup> It showed an increase as well as a blue shift of  $\sim 20$  nm from pure to AA + PGc (Fig. S5a). In FT-IR, the O-H and C=C stretching frequency enhanced following the same trend (Fig. S5b). The zoomed view of the characteristic bands for C=O and C=C are shown separately. In <sup>1</sup>H-NMR spectrum, the intensity of the downfield chemical shift for O-H proton ( $\delta = \sim 15.4$  ppm) and the olefinic proton ( $\delta = \sim 5.5$  ppm) increased. The peak integrals were calculated by fixing the integral for -CH<sub>3</sub> peak at  $\delta = 2.00 - 2.02$  ppm as '1'. The chemical shift of the -CH<sub>3</sub> peak appeared at this position when the AA molecule remained in its enol form. There is also a minor peak at  $\delta = \sim 2.20$  ppm for keto form.<sup>5</sup> Presence of this 'keto' peak in much lower intensity signified that, there were some of the keto molecules in very low concentration but mostly, enol dominated.

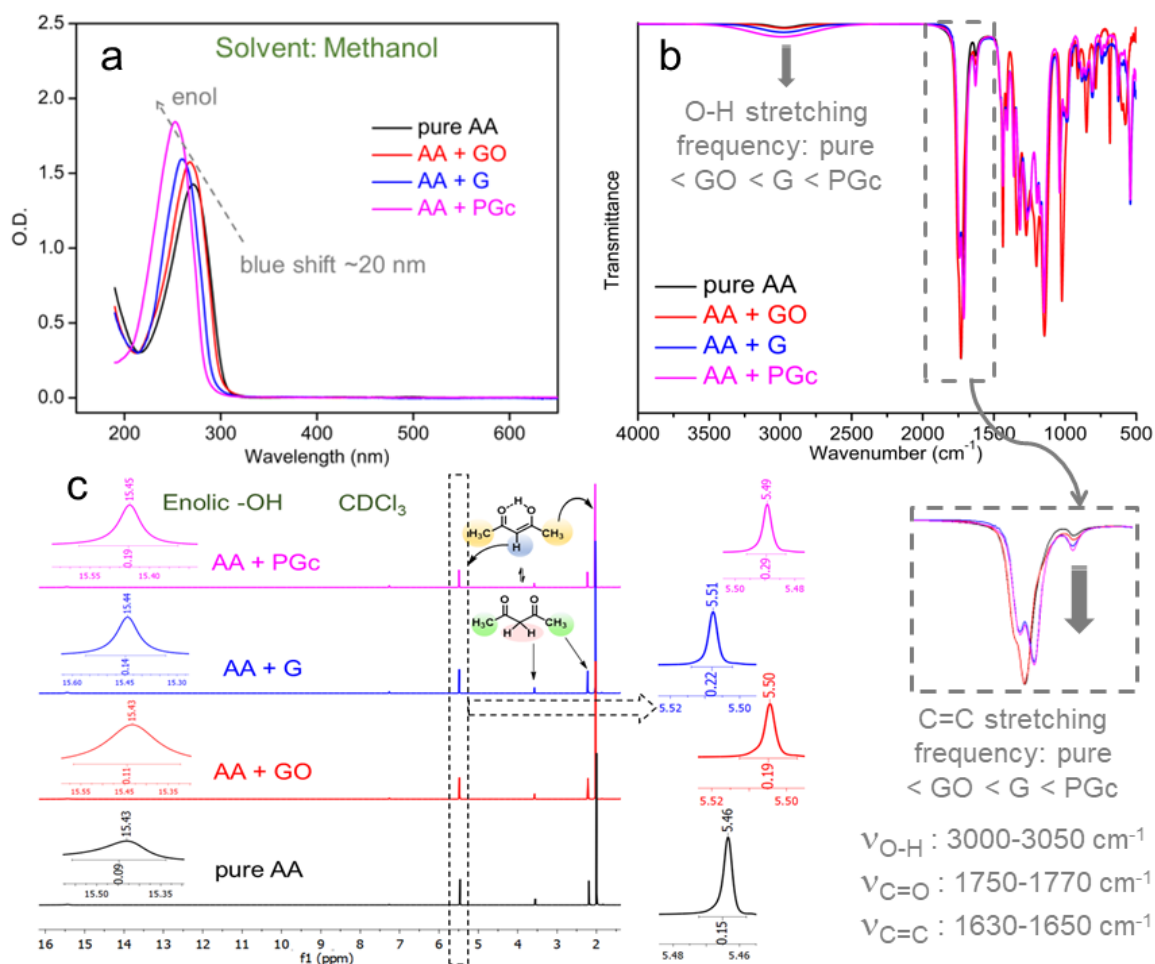


Fig. S5. Spectroscopic analyses of pure AA and its interaction with three graphitic materials: (a) UV-Vis spectrum in methanol, (b) FT-IR spectrum without any solvent, and (c) <sup>1</sup>H-NMR spectrum in CDCl<sub>3</sub>.



The enolization trend in MAA and DMM under the effect of GO, G, and PGc remained the same as for the previous molecules. Fig. S6 represents the UV-Vis, FT-IR, and  $^1\text{H-NMR}$  spectrum of MAA. The spectrum indicated the coexistence of keto and enol tautomer in both solution phase (Fig. S6a, S6c) and solvent-free phase (Fig. S6b), unlike  $\text{CF}_3\text{-DK}$  which was mostly enol-dominated. The extent of enol increased when the adsorbent changed from GO to G to PGc.<sup>6</sup> For DMM, the overall enol-content was very less (Fig. S7). This was strikingly different from the other three  $\beta$ -diketo molecules and was consistent with our theoretical results (Table S3, last column). The UV-Vis spectrum revealed a faint existence of enol tautomer in a polar, protic solvent which increased upon the addition of adsorbents in previously-mentioned sequence (Fig. S7a). In FT-IR spectrum there was no  $\nu_{\text{O-H}}$  and  $\nu_{\text{C=C}}$  in the pure DMM (Fig. S7b). These two peaks emerged upon adsorbent addition, but the evolution of the intensities ( $\text{GO} < \text{G} < \text{PGc}$ ) was quite less compared to the other three molecules. The same trend was observed in  $^1\text{H-NMR}$  spectrum where the olefinic H at  $\delta = \sim 4.7$  ppm (in GO, G, and PGc) was too small to be visualized.<sup>6</sup>

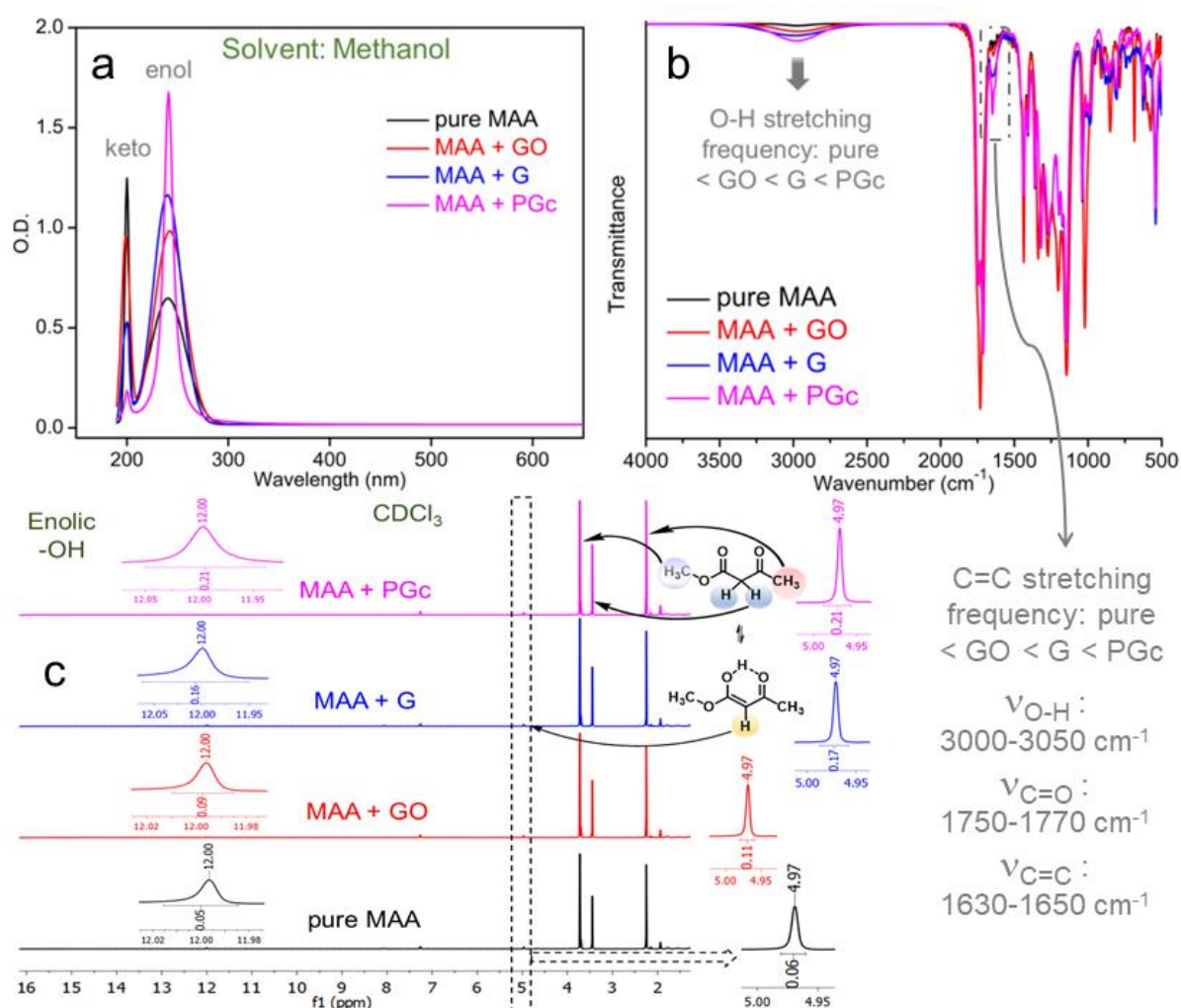


Fig. S6. Spectroscopic analyses of pure MAA and its interaction with three graphitic materials: (a) UV-Vis spectrum in methanol, (b) FT-IR spectrum without any solvent, and (c)  $^1\text{H-NMR}$  spectrum in  $\text{CDCl}_3$ .

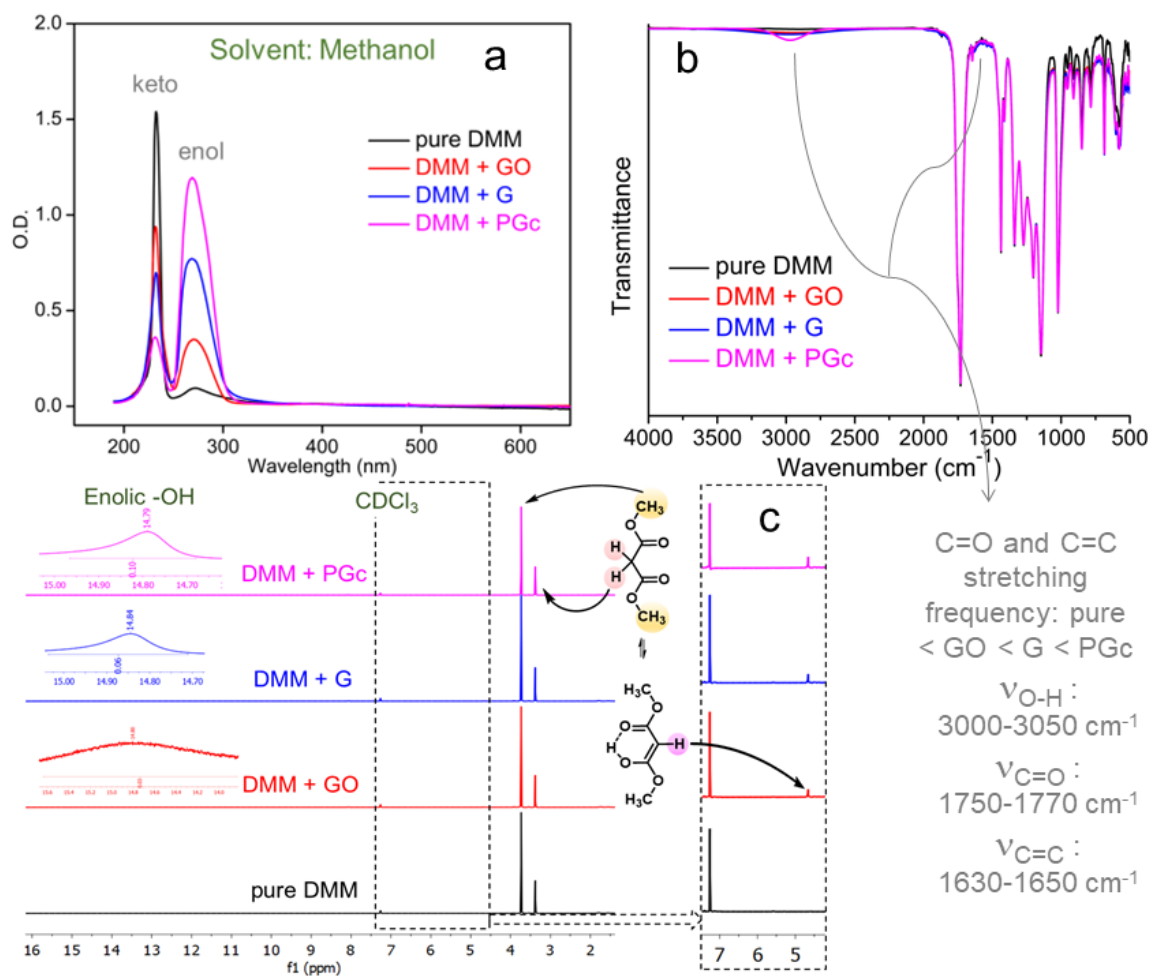


Fig. S7. Spectroscopic analyses of pure DMM and its interaction with three graphitic materials: (a) UV-Vis spectrum in methanol, (b) FT-IR spectrum without any solvent, and (c)  $^1\text{H-NMR}$  spectrum in  $\text{CDCl}_3$ .

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