Supporting Information

One-pot green synthesis of N-acetylglycine from renewable N-acetyl glucosamine

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1. Experimental and computational details

1.1 Materials

NAG (99%), Ag_2O (99%+), WO_3 (99.9%), MoO_3 (99%), CeO_2 (99.99%), Bi_2O_3 (99.99%), Nb_2O_5 (99.99%), acetamide ($AcNH_2$, 98%), glycollic acid (GA, 99%), V_2O_5 (99.5%), formic acid (FA, ACS grade), $NaHCO_3$ (AR), K_2CO_3 (99%), $CaCO_3$ (AR), CH_3COONa (99%) and Co_3O_4 (99.99%) were purchased from Adamas-beta (Shanghai, China). $(NH_4)_2CO_3$ (ACS), Na_2SO_3 (AR), $MgCO_3{\cdot}5H_2O$ (AR), $KHCO_3$ (AR) and Na_2CO_3 (99.95%) were purchased from KESHI (Chengdu China). NaOH (AR), CuO (99%), acetic acid (AA, 99.5%) and AcGly (99%) were purchased from Macklin (Shanghai, China). MgO (AR) was purchased from Greagent (Shanghai, China). MnO_2 (99%) was purchased from Aladdin (Shanghai, China). N-acetyl glucosaminic acid (NAGA) was prepared according to the literature[1].

1.2 Catalytic activity test and product analysis

The catalytic conversion of NAG and other substrates to AcGly was performed in an autoclave equipped with a stirrer. Typically, the reactor was charged with NAG (66 mg, 0.3 mmol), MgO (20 mg, 0.5 mmol), Ag_2O (12 mg, 0.05 mmol), and water (5 mL) in turn. Pressurized O_2 (typically 0.3 MPa) was introduced into the reactor subsequently. The one-pot transformation was carried out in an oil bath for a desired reaction time. Then the reaction was quenched by cold water and O_2 was released. Filtration was conducted before HPLC analysis.

The quantitative analysis of NAG and products was performed by HPLC (Agilent 1260). The HPLC was equipped with Aminex HPX-87H Column (300 × 7.8 mm, 50 °C), a Refractive Index detector (35 °C) and a PDA detector, where a 5 mM H_2SO_4 solution at a flow rate of 0.6 $mL{\cdot}min^{-1}$ was used as the mobile phase. The conversion of NAG and the yields of products were determined based on external standard curves established with authentic samples.

Conversion of NAG (%) = mol of NAG reacted/ mol of starting NAG × 100%.

Yield of AcGly (mol%) = mol of AcGly formed/ mol of starting NAG × 100%.

Yield of $AcNH_2$ (mol%) = mol of $AcNH_2$ formed/ mol of starting NAG× 100%.

Yield of NAGA (mol%) = mol of NAGA formed/ mol of starting NAG× 100%.

Yield of FA (mol%) = mol of FA formed/ mol of starting NAG/ 8 × 100%.

Yield of AA (mol%) = mol of AA formed/ mol of starting NAG/ 4 × 100%.

Yield of GA (mol%) = mol of GA formed/ mol of starting NAG/ 4 × 100%.

1.3 Computational details

A polarized continuum model based on solute electron density (PCM-SMD)[2-3] were applied to simulate the solvent effect of aqueous solution, using self-consistent reaction field (SCRF) method[4-7]. Geometry optimizations for the reactants, products, intermediates (IMs), and transition states (TSs) were run to locate all of the stationary points in aqueous solution without any symmetry constraints. The Minnesota M06 functional method[8-9] with usage of empirical Grimme's D3 dispersion correction (GD3),[10-11] was employed with the def2-SVP basis set[12-13] for all atoms, *i.e.*, M06-GD3/def2-SVP/PCM-SMD(water). Moreover, the stability of the DFT wave-function of the auxiliary Kohn–Sham determinant was examined.[14] Harmonic vibrational frequency calculations were conducted to characterize all stationary point. Herein, minima have zero imaginary frequencies and transition structure (TS) has a unique imaginary frequency. Intrinsic reaction coordinate (IRC) was used to identify transition states connecting two relevant minima.[15] Unless otherwise specified, the relative Gibbs free energies (ΔG, kcal mol^{-1}) are obtained at the level of M06-GD3/def2-SVP/PCM-SMD(water), under experimental temperature and pressure (403.15 K and 1 atm). All density functional theory (DFT) calculations were carried out with the Gaussian 09 programs.[16]

2. Supplementary results and discussions

2.1 The HPLC spectra of NAG and AcGly

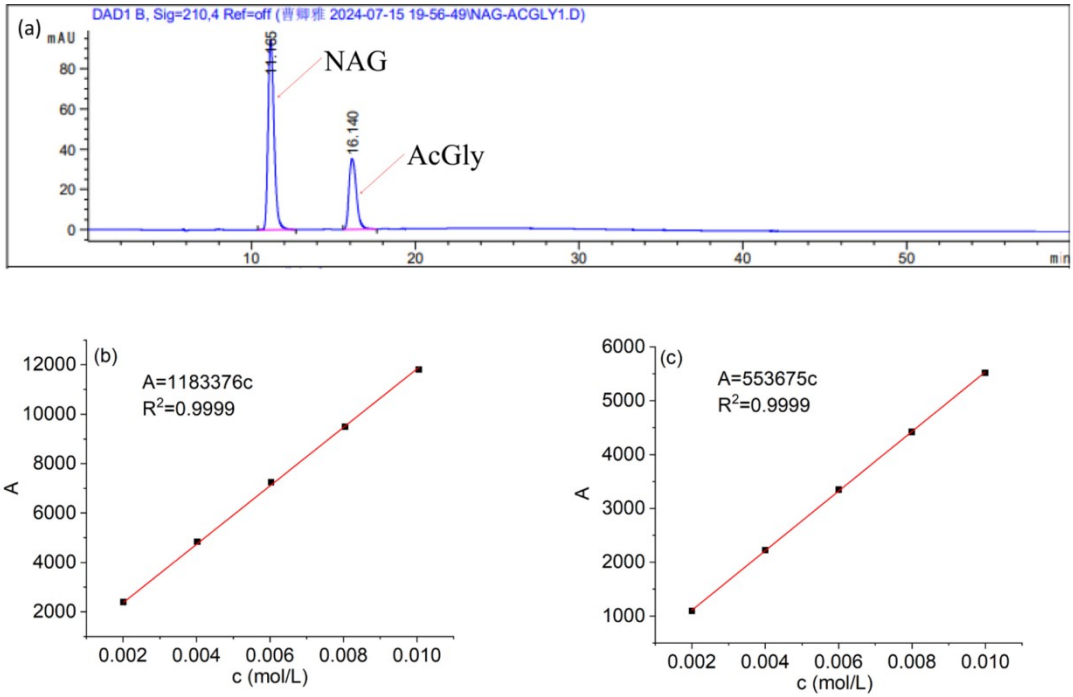


Fig. S2. (a) HPLC spectra of NAG and AcGly; standard curve of (b)NAG and (c) AcGly.

2.2 The recyclability of catalysts

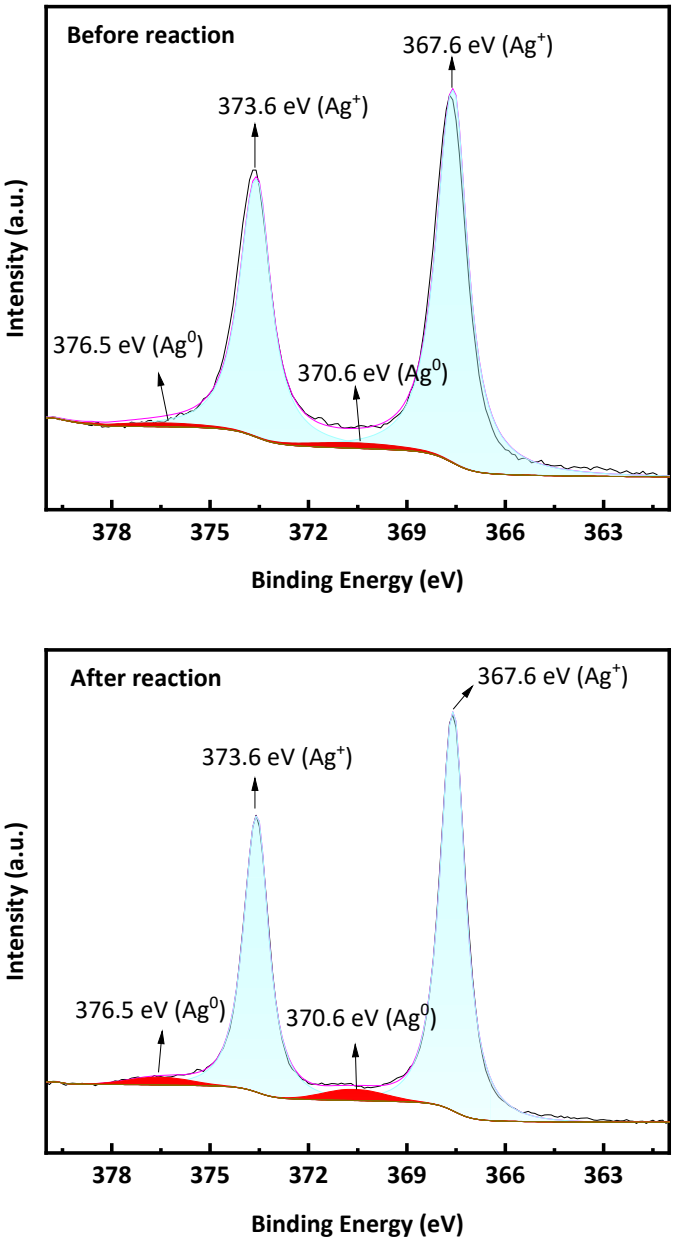


Fig. S2. Deconvoluted Ag 3d XPS spectra of fresh and spent catalysts.

The surface compositions of catalysts were analyzed by XPS. Four peaks (two doublets) are resolvable for the Ag 3d spectra of fresh and spent catalysts. The doublet with the lower binding energy (BE) is from Ag^+. After reaction, the ratio of Ag^+/Ag^0 decreased from 28.5 to 18.3, indicating that slight reduction of Ag_2O occurred during reaction.

2.3 Possible reaction pathways

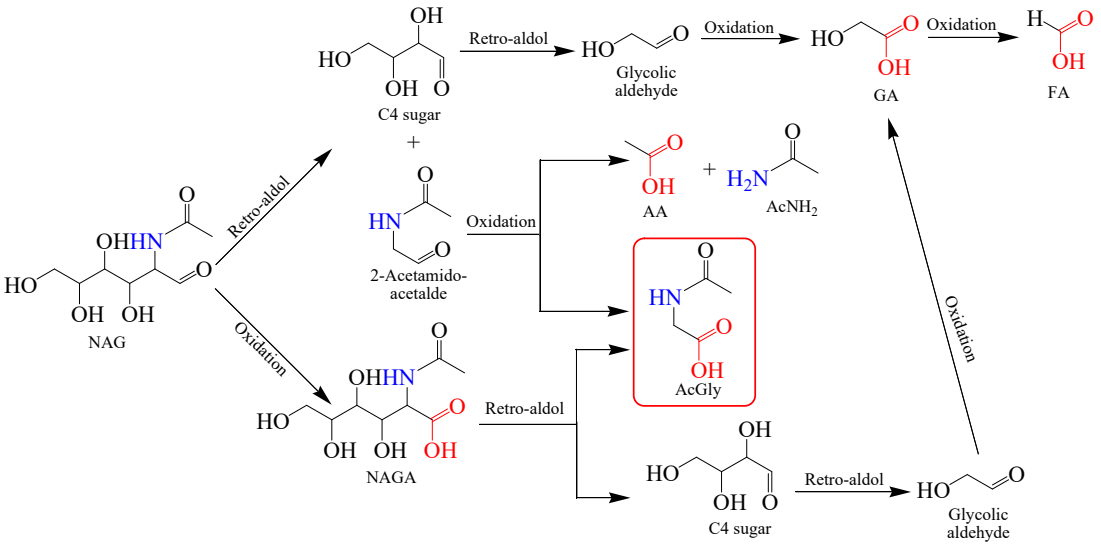
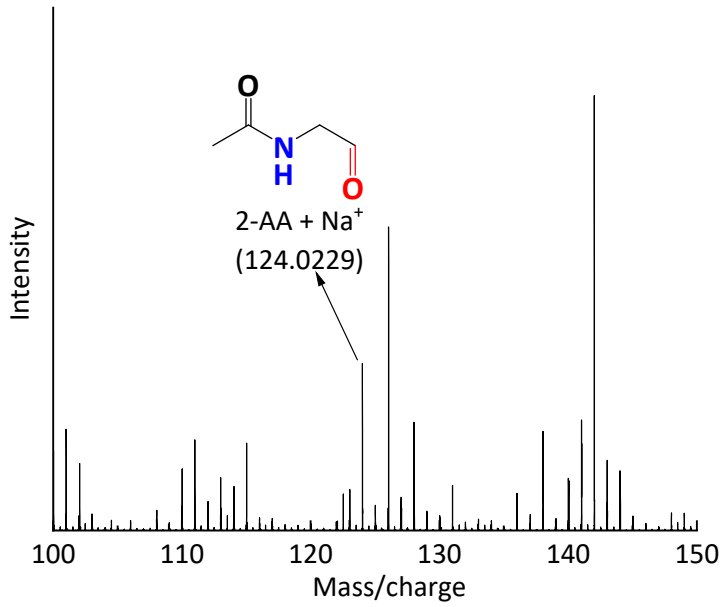


Fig. S3. Possible reaction pathways for the conversion of NAG to identified products.

LC-MS(+)



LC-MS(-)

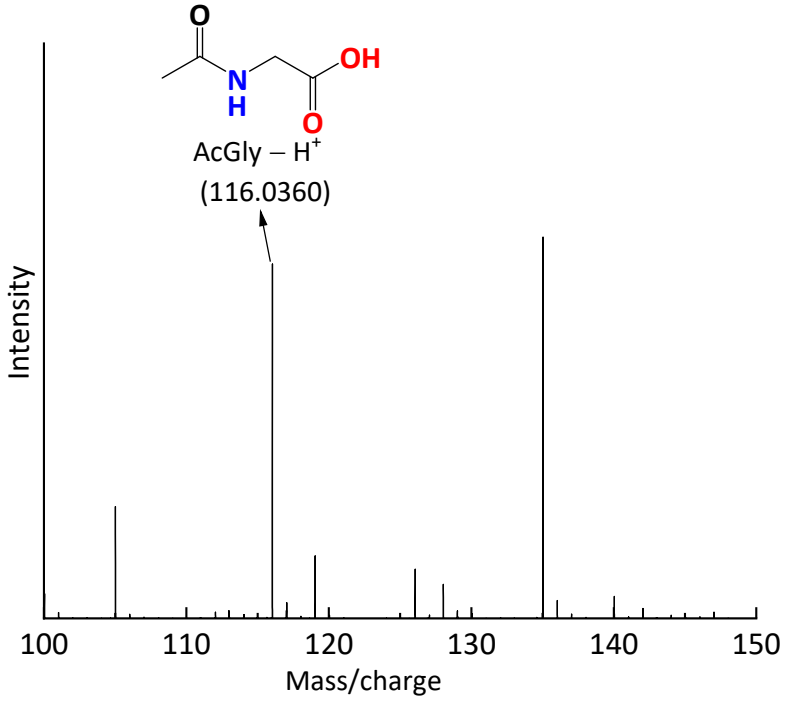


Fig. S4. LC-MS spectra of reaction mixtures after 1 h.

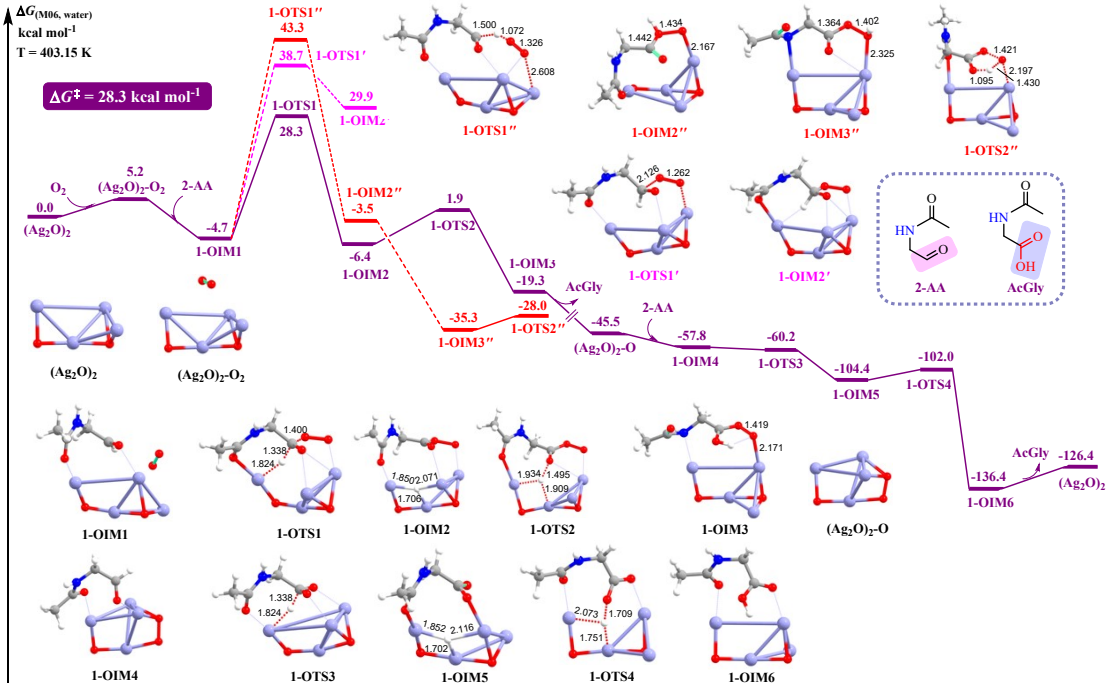


Fig. S5. Gibbs free energy profiles with DFT-optimized structures for the Ag-catalyzed oxidation of **2-AA** to **AcGly**. Selected bond lengths are reported in Å.

The $(Ag_2O)_2$ cluster are employed as the model of reaction catalyst in the current system[17-18]

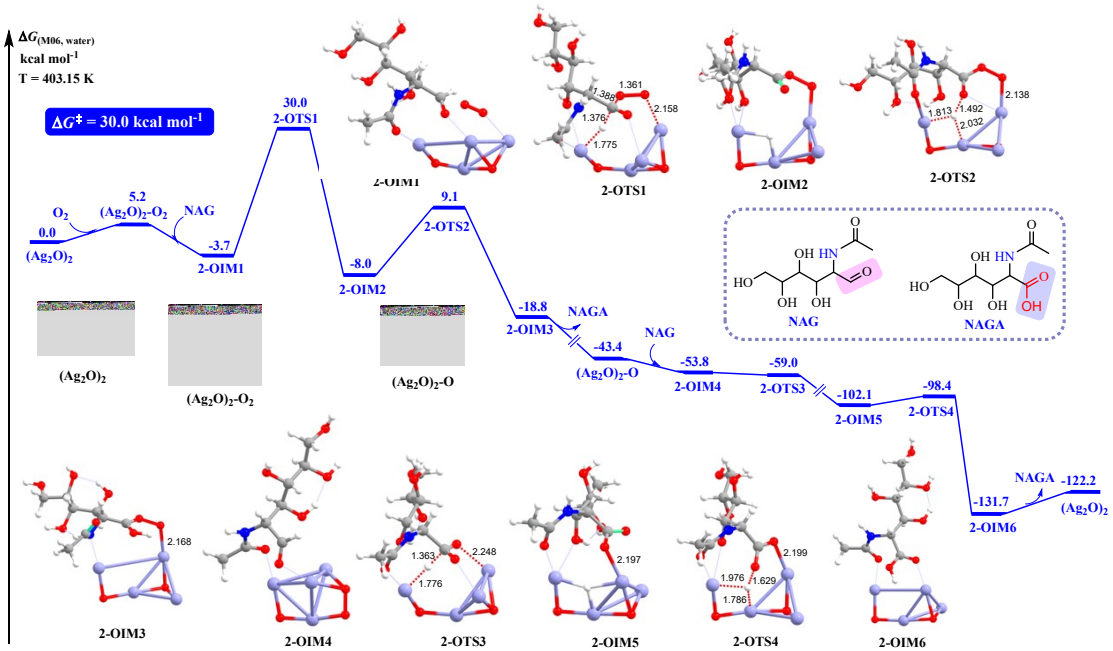


Fig. S6. Gibbs free energy profiles with DFT-optimized structures for the Ag-catalyzed oxidation of **NAG** to **NAGA**. Selected bond lengths are reported in Å.

Table S1. Zero-point energies (*ZPE*, hartree), thermal correction to Gibbs free energy (G_0, hartree), total energies (E_c, hartree) corrected by the addition of *ZPE*, sum of electronic and thermal free energies (G_c, hartree) with the addition of *ZPE* and thermal corrections, and relative energies (ΔE, kcal mol^{-1}) and relative Gibbs free energies (ΔG, kcal mol^{-1}) of various species with respect to initial reactions for the Mg-catalyzed C–C bond cleavage of NAG under experimental temperature and pressure (403.15 K and 1 atm). IF is imaginary frequency.

Species	*ZPE*	E_c	G_0	G_c	ΔE	ΔG	IF
NAG	0.24497	-818.70104	0.17569	-818.77032			
$Mg(OH)(H_2O)_3^+$	0.08564	-504.72659	0.03022	-504.78200			
NAG + $Mg(OH)(H_2O)_3^+$	0.33060	-1323.42763	0.20591	-1323.55232	0.0	0.0	
1-IM1	0.28422	-1170.77611	0.20006	-1170.86027			
H_2O	0.02129	-76.31533	-0.00502	-76.34164			
1-IM1 + 2 H_2O	0.32681	-1323.40676	0.19002	-1323.54355	13.1	5.5	
1-TS1	0.28000	-1170.77121	0.19877	-1170.85244			839.64*i*
1-TS1 + 2 H_2O	0.32258	-1323.40187	0.18873	-1323.53573	16.2	10.4	
1-IM2	0.28360	-1170.80264	0.20171	-1170.88453			
1-IM2 + 2 H_2O	0.32619	-1323.43330	0.19167	-1323.56782	-3.6	-9.7	
1-TS2	0.28062	-1170.77913	0.19692	-1170.86284			244.18*i*
1-TS2 + 2 H_2O	0.32321	-1323.40979	0.18688	-1323.54612	11.2	3.9	
1-IM3	0.15091	-713.35402	0.08686	-713.41807			
C4	0.12805	-457.40692	0.07723	-457.45774			
1-IM3 + **C4** + $2H_2O$	0.32155	-1323.39160	0.15405	-1323.55909	22.6	-4.2	
1-TS3′	0.14684	-713.32218	0.08779	-713.38124			1850.40*i*
1-TS3′ + **C4** + $2H_2O$	0.31748	-1323.35976	0.15498	-1323.52226	42.6	18.9	
1-TS3	0.17088	-789.66741	0.10382	-789.73446			1781.64*i*
1-TS3 + **C4** + H_2O	0.32022	-1323.38965	0.17603	-1323.53384	23.8	11.6	
1-IM4	0.15044	-713.34160	0.08576	-713.40628			

1-IM4 + **C4** + $2H_2O$	0.32108	-1323.37917	0.15295	-1323.54730	30.4	3.1
2-AA	0.11088	-361.26456	0.06242	-361.31303		
C4 + **2-AA** + $Mg(OH)(H_2O)_3^+$	0.32457	-1323.39807	0.16987	-1323.55277	18.5	-0.3

Table S2. Zero-point energies (*ZPE*, hartree), thermal correction to Gibbs free energy (G_0, hartree), total energies (E_c, hartree) corrected by the addition of *ZPE*, sum of electronic and thermal free energies (G_c, hartree) with the addition of *ZPE* and thermal corrections, and relative energies (ΔE, kcal mol^{-1}) and relative Gibbs free energies (ΔG, kcal mol^{-1}) of various species with respect to initial reactions for the Ag-catalyzed oxidation of **2-AA** under experimental temperature and pressure (403.15 K and 1 atm). IF is imaginary frequency.

Species	*ZPE*	E_c	G_0	G_c	ΔE	ΔG	IF
2-AA	0.11088	-361.26456	0.06242	-361.31303			
$(Ag_2O)_2$	0.00593	-738.26844	-0.05601	-738.33038			
O_2	0.00400	-150.12824	-0.02432	-150.15656			
2*2-AA + **$(Ag_2O)_2$** + O_2	0.23170	-1610.92581	0.04452	-1611.11300	0.0	0.0	
$(Ag_2O)_2$-O_2	0.01067	-888.40477	-0.06327	-888.47871			
2*2-AA + **$(Ag_2O)_2$-O_2**	0.23244	-1610.93389	0.06156	-1611.10477	-5.1	5.2	
1-OIM1	0.12405	-1249.71469	0.03124	-1249.80751			
1-OIM1 + **2-AA**	0.23494	-1610.97926	0.09366	-1611.12054	-33.5	-4.7	
1-OTS1″	0.11981	-1249.64476	0.03359	-1249.73097			518.09*i*
1-OTS1" + **2-AA**	0.23069	-1610.90932	0.09601	-1611.04400	10.3	43.3	
1-OIM2″	0.12764	-1249.72356	0.04558	-1249.80563			
1-OIM2″ + **2-AA**	0.23853	-1610.98813	0.10800	-1611.11866	-39.1	-3.5	
1-OIM3″	0.12789	-1249.76950	0.04113	-1249.85627			
1-OIM3" + **2-AA**	0.23878	-1611.03407	0.10355	-1611.16929	-67.9	-35.3	

1-OTS2′	0.12524	-1249.76125	0.04196	-1249.84453			882.64*i*
1-OTS2″ + **2-AA**	0.23613	-1611.02581	0.10438	-1611.15756	-62.8	-28.0	
1-OTS1′	0.12397	-1249.65350	0.03919	-1249.73829			121.78*i*
1-OTS1′ + **2-AA**	0.23486	-1610.91807	0.10161	-1611.05132	4.9	38.7	
1-OIM2′	0.12525	-1249.67191	0.04487	-1249.75229			
1-OIM2′ + **2-AA**	0.23613	-1610.93648	0.10729	-1611.06532	-6.7	29.9	
1-OTS1	0.12098	-1249.67454	0.04063	-1249.75489			824.41*i*
1-OTS1 + **2-AA**	0.23187	-1610.93911	0.10305	-1611.06792	-8.3	28.3	
1-OIM2	0.12182	-1249.72694	0.03857	-1249.81020			

Continued Table S2

Species	*ZPE*	E_c	G_0	G_c	ΔE	ΔG	IF
1-OIM2 + **2-AA**	0.23270	-1610.99151	0.10099	-1611.12323	-41.2	-6.4	
1-OTS2	0.12019	-1249.71471	0.03792	-1249.79698			1227.62*i*
1-OTS2 + **2-AA**	0.23107	-1610.97928	0.10033	-1611.11001	-33.6	1.9	
1-OIM3	0.12825	-1249.74683	0.04430	-1249.83078			
1-OIM3 + **2-AA**	0.23913	-1611.01140	0.10672	-1611.14381	-53.7	-19.3	
$(Ag_2O)_2$-O	0.00878	-813.31725	-0.05437	-813.38040			
AcGly	0.11655	-436.43914	0.06363	-436.49206			
$(Ag_2O)_2$-O + AcGly + **2-AA**	0.23622	-1611.02096	0.07168	-1611.18549	-59.7	-45.5	
1-OIM4	0.12184	-1174.63055	0.03938	-1174.71302			
1-OIM4 + AcGly	0.23840	-1611.06969	0.10301	-1611.20508	-90.3	-57.8	
1-OTS3	0.11533	-1174.63639	0.03479	-1174.71693			364.58*i*
1-OTS3 + **AcGly**	0.23189	-1611.07553	0.09842	-1611.20900	-94.0	-60.2	

1-OIM5	0.11810	-1174.70409	0.03490	-1174.78730			
1-OIM5 + AcGly	0.23466	-1611.14324	0.09853	-1611.27936	-136.4	-104.4	
1-OTS4	0.11596	-1174.70268	0.03509	-1174.78355			575.81*i*
1-OTS4 + AcGly	0.23252	-1611.14183	0.09872	-1611.27562	-135.6	-102.0	
1-OIM6	0.12554	-1174.75711	0.04428	-1174.83837			
1-OIM6 + AcGly	0.24209	-1611.19625	0.10791	-1611.33043	-169.7	-136.4	
2AcGly + **$(Ag_2O)_2$**	0.23903	-1611.14673	0.07126	-1611.31451	-138.6	-126.4	

Table S3. Zero-point energies (*ZPE*, hartree), thermal correction to Gibbs free energy (G_0, hartree), total energies (E_c, hartree) corrected by the addition of *ZPE*, sum of electronic and thermal free energies (G_c, hartree) with the addition of *ZPE* and thermal corrections, and relative energies (ΔE, kcal mol^{-1}) and relative Gibbs free energies (ΔG, kcal mol^{-1}) of various species with respect to initial reactions for the Ag-catalyzed oxidation of **NAG** under experimental temperature and pressure (403.15 K and 1 atm). IF is imaginary frequency.

Species	*ZPE*	E_c	G_0	G_c	ΔE	ΔG	IF
NAG	0.24497	-818.70104	0.17569	-818.77032			
$(Ag_2O)_2$	0.00593	-738.26844	-0.05601	-738.33038			
O_2	0.00400	-150.12824	-0.02432	-150.15656			
2NAG + **$(Ag_2O)_2$** + O_2	0.49986	-2525.79876	0.27105	-2526.02757	0.0	0.0	
$(Ag_2O)_2$-O_2	0.01067	-888.40477	-0.06327	-888.47871			
2NAG + **$(Ag_2O)_2$-O_2**	0.50060	-2525.80684	0.28810	-2526.01935	-5.1	5.2	
2-OIM1	0.25838	-1707.15424	0.14941	-1707.26321			
2-OIM1 + NAG	0.50334	-2525.85528	0.32510	-2526.03353	-35.5	-3.7	
2-OTS1	0.25386	-1707.10772	0.15207	-1707.20951			811.03*i*
2-OTS1 + NAG	0.49883	-2525.80876	0.32776	-2525.97983	-6.3	30.0	
2-OIM2	0.25555	-1707.16449	0.14999	-1707.27005			
2-OIM2 + NAG	0.50052	-2525.86553	0.32568	-2526.04037	-41.9	-8.0	
2-OTS2	0.25450	-1707.14424	0.15595	-1707.24278			1269.83*i*
2-OTS2 + NAG	0.49947	-2525.84527	0.33164	-2526.01310	-29.2	9.1	
2-OIM3	0.26090	-1707.18320	0.15683	-1707.28727			
2-OIM3 + NAG	0.50587	-2525.88424	0.33252	-2526.05759	-53.6	-18.8	
$(Ag_2O)_2$-O	0.00878	-813.31725	-0.05437	-813.38040			
NAGA	0.25098	-893.87532	0.18032	-893.94597			
$(Ag_2O)_2$-O + NAGA + NAG	0.50473	-2525.89360	0.30164	-2526.09669	-59.5	-43.4	
2-OIM4	0.25568	-1632.06590	0.15427	-1632.16732			
2-OIM4 + NAGA	0.50666	-2525.94122	0.33459	-2526.11329	-89.4	-53.8	

2-OTS3	0.24907	-1632.07653	0.14997	-1632.17562			336.51*i*
2-OTS3 + NAGA	0.50005	-2525.95184	0.33030	-2526.12160	-96.1	-59.0	

Continued Table S3

Species	*ZPE*	E_c	G_0	G_c	ΔE	ΔG	IF
2-OIM5	0.25124	-1632.14144	0.14844	-1632.24423			
2-OIM5 + NAGA	0.50222	-2526.01675	0.32877	-2526.19020	-136.8	-102.1	
2-OTS4	0.24988	-1632.13830	0.14984	-1632.23834			775.91*i*
2-OTS4 + NAGA	0.50086	-2526.01362	0.33017	-2526.18431	-134.8	-98.4	
2-OIM6	0.25833	-1632.18802	0.15485	-1632.29151			
2-OIM6 + NAGA	0.50931	-2526.06334	0.33517	-2526.23748	-166.0	-131.7	
2NAGA + **$(Ag_2O)_2$**	0.50789	-2526.01907	0.30464	-2526.22232	-138.2	-122.2	

Table S4. Zero-point energies (*ZPE*, hartree), thermal correction to Gibbs free energy (G_0, hartree), total energies (E_c, hartree) corrected by the addition of *ZPE*, sum of electronic and thermal free energies (G_c, hartree) with the addition of *ZPE* and thermal corrections, and relative energies (ΔE, kcal mol^{-1}) and relative Gibbs free energies (ΔG, kcal mol^{-1}) of various species with respect to initial reactions for the Mg-catalyzed C–C bond cleavage of NAGA under experimental temperature and pressure (403.15 K and 1 atm). IF is imaginary frequency.

Species	*ZPE*	E_c	G_0	G_c	ΔE	ΔG	IF
NAGA	0.25098	-893.87532	0.18032	-893.94597			
$Mg(OH)(H_2O)_3^+$	0.08564	-504.72659	0.03022	-504.78200			
NAGA + $Mg(OH)(H_2O)_3^+$	0.33662	-1398.60191	0.21055	-1398.72798	0.0	0.0	
2-IM1	0.29000	-1245.95325	0.20372	-1246.03954			
H_2O	0.02129	-76.31533	-0.00502	-76.34164			
2-IM1 + 2 H_2O	0.33259	-1398.58391	0.19368	-1398.72283	11.3	3.2	
2-TS1	0.28583	-1245.94795	0.20223	-1246.03154			804.96*i*
2-TS1 + 2 H_2O	0.32841	-1398.57860	0.19219	-1398.71482	14.6	8.3	
2-IM2	0.28936	-1245.97957	0.20493	-1246.06400			
2-IM2 + 2 H_2O	0.33194	-1398.61023	0.19489	-1398.74728	-5.2	-12.1	
2-TS2	0.28550	-1245.94452	0.20031	-1246.02971			218.49*i*
2-TS2 + 2 H_2O	0.32809	-1398.57518	0.19027	-1398.71300	16.8	9.4	
2-IM3	0.15587	-788.51010	0.09043	-788.57553			
C4	0.12805	-457.40692	0.07723	-457.45774			
2-IM3 + **C4** + $2H_2O$	0.32650	-1398.54767	0.15762	-1398.71656	34.0	7.2	
2-TS3′	0.15249	-788.49480	0.09123	-788.55606			1546.20*i*
2-TS3′ + **C4** + $2H_2O$	0.32313	-1398.53238	0.15842	-1398.69709	43.6	19.4	
2-TS3	0.17683	-864.83941	0.10827	-864.90797			1634.63*i*
2-TS3 + **C4** + H_2O	0.32617	-1398.56166	0.18048	-1398.70736	25.3	12.9	
2-IM4	0.15619	-788.52031	0.08943	-788.58707			
2-IM4 + **C4**	0.32683	-1398.55788	0.15662	-1398.72810	27.6	-0.1	

+ $2H_2O$						
AcGly	0.11655	-436.43914	0.06363	-436.49206		
C4 + **AcGly** + $Mg(OH)(H_2O)_3^+$	0.33024	-1398.57265	0.17108	-1398.73181	18.4	-2.4

Cartesian coordinates of all optimized structures of the stationary points.

NAG

6	-3.632928	-0.426368	0.560226
6	-2.430385	-0.112373	-0.293222
6	-1.297962	-1.116062	-0.123047
6	0.032307	-0.651054	-0.728465
6	-0.023708	-0.172602	-2.193916
6	-0.621184	1.203275	-2.392823
8	-1.916380	1.160933	0.048261
8	-4.589392	0.574990	0.301959
8	-1.627671	-2.355764	-0.711590
1	-5.280614	0.522277	0.974853
1	-1.245445	-1.845523	-2.632182
1	-4.016524	-1.436451	0.314439
1	-1.098202	-1.236445	0.962464
1	1.036742	-0.017229	-2.483063
1	-3.321831	-0.432480	1.623905
8	0.656498	0.311712	0.082220
1	0.676010	-1.549072	-0.730895
1	-2.355093	-2.762578	-0.220719
1	-0.025815	0.965434	0.314696
1	-2.755187	-0.121699	-1.356711
8	-1.523469	1.452454	-3.157222
7	-0.607586	-1.168004	-3.051174
6	-0.396620	-1.161321	-4.386594
8	0.351877	-0.345865	-4.924630
6	-1.133391	-2.202043	-5.170607
1	-1.605803	-2.967834	-4.540632
1	-1.913539	-1.703089	-5.767049
1	-0.438823	-2.677400	-5.878279
1	-2.661685	1.781375	0.077120
1	-0.102164	2.009339	-1.820903

$Mg(OH)(H_2O)_3^+$

12	1.262840	-0.667666	-0.100718
8	-0.262658	-1.755568	-0.192191
1	-0.441208	-2.271843	-0.983228
8	1.263003	0.224443	1.727816
1	1.701366	1.075425	1.877879
8	1.550797	0.882606	-1.390740
1	1.737947	0.681279	-2.320555
8	3.072054	-1.602686	-0.234894
1	3.161426	-2.474759	0.178642
1	0.428633	0.271785	2.218606
1	0.854634	1.557607	-1.417591
1	3.872829	-1.118402	0.018746

1-IM1

6	-3.750488	-0.800460	0.542553
6	-2.658727	-0.218920	-0.319953
6	-1.296630	-0.846787	-0.055476
6	-0.126532	-0.046505	-0.631781
6	-0.192547	0.307513	-2.137463
6	-0.975729	1.559980	-2.435095
8	-2.533023	1.168203	-0.061567
8	-4.927714	-0.093854	0.229641
8	-1.203565	-2.145196	-0.590575
1	-5.586793	-0.273635	0.912627
1	-0.909554	-1.667929	-2.503031
1	-3.851009	-1.885812	0.345117
1	-1.127326	-0.857290	1.041935
1	0.847220	0.588579	-2.407217
1	-3.467893	-0.674200	1.606477
8	0.089844	1.133599	0.129085
1	0.760137	-0.690249	-0.509776
1	-1.807903	-2.736561	-0.120702
1	-0.795177	1.427742	0.442908
1	-2.932880	-0.384546	-1.384253
8	-0.543965	2.661095	-2.123957
7	-0.617786	-0.797266	-2.950309
6	-0.631762	-0.628346	-4.291556
8	-0.324687	0.460380	-4.782936
6	-1.024678	-1.805007	-5.120066

1	-1.338875	-2.669028	-4.519863
1	-1.838233	-1.508092	-5.798108
1	-0.168088	-2.092743	-5.748890
1	-3.427702	1.532351	0.041765
1	-1.963084	1.462946	-2.936114
12	0.895096	2.943514	-0.621911
8	2.732897	2.487913	-1.347462
1	3.430389	2.285079	-0.704918
8	0.554231	4.176679	0.740336
1	0.797205	5.100154	0.628324
1	2.825957	1.822716	-2.046835

1-TS1

6	-3.671457	-0.472715	0.526005
6	-2.531175	-0.058471	-0.370281
6	-1.218382	-0.732719	0.002405
6	0.036249	-0.135928	-0.648355
6	-0.097712	0.244639	-2.141006
6	-0.839868	1.530707	-2.393897
8	-2.342403	1.336869	-0.298579
8	-4.826255	0.178855	0.051854
8	-1.245827	-2.094037	-0.378800
1	-5.523666	0.090706	0.714596
1	-0.958494	-1.680472	-2.441152
1	-3.787689	-1.574934	0.511477
1	-1.065190	-0.632010	1.098042
1	0.939323	0.475869	-2.464033
1	-3.428541	-0.174194	1.565359
8	0.593996	0.925867	0.060372
1	0.755300	-0.978566	-0.645189
1	-1.974028	-2.540199	0.075917
1	-0.006600	1.614101	0.690274
1	-2.792157	-0.356563	-1.409355
8	-0.359469	2.620938	-2.108837
7	-0.621831	-0.844381	-2.920869
6	-0.669487	-0.725906	-4.266781
8	-0.299177	0.313115	-4.817192
6	-1.177410	-1.903873	-5.030595
1	-1.524016	-2.721109	-4.384337
1	-1.997900	-1.576795	-5.686252
1	-0.370868	-2.273775	-5.682212
1	-3.204399	1.751152	-0.460987
1	-1.828026	1.469936	-2.898543
12	0.975808	2.935933	-0.547291
8	2.728025	2.956459	-1.556079
1	3.570707	2.903887	-1.079476
8	-0.107083	2.909045	1.102966
1	-1.024602	3.194976	1.026197
1	2.804929	2.319610	-2.284413

1-IM2

6	-3.294835	-0.291400	0.749849
6	-2.122779	0.146860	-0.098263
6	-1.063783	-0.935287	-0.263097
6	0.181311	-0.516501	-1.068120
6	-0.124856	-0.048939	-2.527254
6	-0.847959	1.259294	-2.663815
8	-1.549728	1.294885	0.516927
8	-4.116186	0.842709	0.908113
8	-1.640697	-2.068051	-0.881985
1	-4.690561	0.707679	1.673175
1	-1.289670	-1.786333	-2.837903
1	-3.828923	-1.121358	0.251980
1	-0.683286	-1.192051	0.747109
1	0.878718	0.172297	-2.947161
1	-2.914910	-0.659287	1.723249
8	0.931149	0.413697	-0.406740
1	0.728490	-1.477534	-1.223583
1	-2.171481	-2.559687	-0.240576
1	-2.521187	0.421046	-1.103042
8	-0.604372	2.264114	-2.011403
7	-0.750441	-1.071968	-3.326815
6	-0.642463	-1.076298	-4.674196
8	-0.017791	-0.201215	-5.275336
6	-1.318754	-2.203126	-5.389099
1	-1.834029	-2.901622	-4.716185
1	-2.042003	-1.785711	-6.105908
1	-0.565141	-2.750910	-5.975277
1	-2.295659	1.840431	0.830450
1	-1.643117	1.296414	-3.445203

12	0.265799	2.200445	-0.085428
8	2.076472	3.142547	-0.346648
1	2.295344	3.965402	0.115157
8	-0.430869	3.934992	0.766847
1	-0.014149	4.777937	0.532135
1	2.889090	2.615626	-0.340674
1	-1.384781	4.105839	0.758881

1-TS2

6	-3.228085	-0.249120	1.019547
6	-2.137209	0.249526	0.103327
6	-1.213592	-0.876220	-0.350342
6	0.119494	-0.496727	-0.959170
6	-0.288334	0.251171	-3.074101
6	-1.009071	1.349118	-2.642869
8	-1.408218	1.261875	0.795302
8	-3.981092	0.882288	1.389931
8	-1.901206	-1.720993	-1.237653
1	-4.490313	0.672098	2.183853
1	-1.674293	-1.282944	-3.348451
1	-3.836684	-1.005682	0.489862
1	-0.894707	-1.436738	0.558171
1	0.800827	0.318987	-3.172806
1	-2.764589	-0.736235	1.899512
8	0.837751	0.401635	-0.470435
1	0.575867	-1.343668	-1.512047
1	-2.342597	-2.423413	-0.741286
1	-2.612079	0.689205	-0.796566
8	-0.528206	2.331734	-1.979565
7	-0.909067	-0.788360	-3.806244
6	-0.371061	-1.314060	-4.930964
8	0.632656	-0.839214	-5.465690
6	-1.066083	-2.517921	-5.487896
1	-1.991223	-2.777168	-4.955345
1	-1.291804	-2.338723	-6.549830
1	-0.376419	-3.375743	-5.447383
1	-2.071753	1.793210	1.274409
1	-2.107799	1.316283	-2.821518
12	0.185808	2.305812	-0.099297
8	2.072533	3.077963	-0.247864
1	2.356253	3.795829	0.337663
8	-0.475290	4.057558	0.749726
1	-0.157055	4.888897	0.365967
1	2.822517	2.465807	-0.290569
1	-1.433912	4.168871	0.840780

1-IM3

6	-1.001173	0.221472	-2.589676
6	-0.036856	0.830923	-1.855635
1	-1.582173	-0.272811	-4.520488
1	-2.039022	0.274256	-2.250762
8	1.240396	0.941230	-2.099352
7	-0.837376	-0.428595	-3.841995
6	0.093537	-1.304641	-4.213499
8	1.037961	-1.657304	-3.460831
6	-0.008244	-1.888622	-5.578916
1	-0.905233	-1.569895	-6.125511
1	0.887644	-1.604301	-6.152670
1	0.001434	-2.985652	-5.491446
1	-0.411758	1.300746	-0.923895
12	2.373202	-0.575436	-2.474903
8	3.107254	-1.896027	-1.129510
1	3.659583	-1.590565	-0.393627
8	3.956596	-0.107288	-3.649711
1	4.294833	-0.776102	-4.264797
1	3.946665	0.722401	-4.150751
1	2.498080	-2.543496	-0.742276

C4

6	-3.591727	-0.360785	0.515800
6	-2.250419	0.159953	0.072814
6	-1.285207	-0.983198	-0.262287
6	0.039330	-0.464343	-0.755808
8	-1.717838	0.948801	1.111971
8	-4.457040	0.733764	0.701008
8	-1.774787	-1.864020	-1.240734
1	-5.315601	0.389239	0.977770
1	-3.975238	-1.060946	-0.249903
1	-1.052935	-1.509861	0.691155
1	-3.447163	-0.937154	1.454007
8	0.550126	0.572846	-0.396522

1	-2.313958	-2.541533	-0.811475
1	-2.402275	0.763385	-0.850094
1	-0.839476	1.240109	0.813055
1	0.536277	-1.134610	-1.500732

1-TS3′

6	-0.499744	-0.462511	-2.253389
6	0.360951	0.591223	-1.811372
1	-1.632838	-0.637941	-3.997442
1	-1.466588	-0.494748	-1.741946
8	1.470596	0.850556	-2.316999
7	-0.675268	-0.732164	-3.665153
6	0.213624	-1.104237	-4.586343
8	1.435661	-1.258846	-4.357267
6	-0.297548	-1.344008	-5.964737
1	-1.381393	-1.202305	-6.062014
1	0.225996	-0.666309	-6.656022
1	-0.031686	-2.370972	-6.258237
1	0.081562	1.068394	-0.845783
12	2.561193	-0.905555	-2.750128
8	1.470389	-2.087864	-1.616583
1	1.623058	-2.119468	-0.663305
8	4.387146	-0.423057	-3.464773
1	4.450320	0.239913	-4.169836
1	5.092394	-0.198849	-2.838218
1	0.324888	-1.375420	-1.772332

1-TS3

6	-1.090734	-0.506492	-2.572325
6	-0.277356	0.548331	-2.049007
1	-1.747508	-0.840375	-4.526558
1	-2.154192	-0.414237	-2.330441
8	0.936958	0.681734	-2.290075
7	-0.924176	-0.950851	-3.939067
6	0.134783	-1.506178	-4.532372
8	1.232295	-1.699922	-3.966578
6	-0.024228	-1.905666	-5.960489
1	0.723177	-1.365337	-6.561136
1	0.207474	-2.978089	-6.048092
1	-1.026646	-1.713791	-6.364761
1	-0.740695	1.157488	-1.240605
12	1.984449	-1.171440	-2.142466
8	2.957108	-0.674144	-0.378266
1	3.549576	0.092882	-0.383213
8	3.805063	-0.897138	-3.051409
1	4.637246	-1.025087	-2.572226
1	3.952913	-1.265152	-3.935309
1	-0.506613	-1.382591	-1.793957
8	0.486819	-2.108315	-1.201773
1	2.403060	-0.559741	0.408090
1	0.324931	-3.009573	-1.508732

1-IM4

6	-0.776071	-0.302852	-2.406758
6	0.151441	0.850394	-2.118630
1	-1.592675	-0.338217	-4.373457
1	-1.797879	-0.055126	-2.097179
8	1.357632	0.705442	-2.033996
7	-0.786047	-0.621454	-3.820796
6	0.180721	-1.319323	-4.425458
8	1.208195	-1.686537	-3.818616
6	-0.011687	-1.673173	-5.854994
1	-0.946429	-1.282519	-6.276054
1	0.845411	-1.293171	-6.430498
1	0.001225	-2.770491	-5.941172
1	-0.289503	1.863137	-2.002636
12	2.454940	-1.080930	-2.364984
8	2.597939	-1.841745	-0.661400
1	3.138193	-2.621184	-0.503935
8	4.002531	-0.098097	-3.256373
1	4.624083	-0.589805	-3.814492
1	3.782282	0.698570	-3.763950
1	-0.431588	-1.177086	-1.826500

2-AA

6	-0.192708	-0.200085	-2.317366
6	-0.854232	1.111316	-2.610461
1	-1.416647	-1.869314	-2.769766
1	0.894670	-0.046684	-2.442927
8	-1.693914	1.281696	-3.461878
7	-0.658504	-1.291551	-3.121343
6	-0.314385	-1.395904	-4.426950

8	0.514333	-0.646824	-4.942497
6	-1.003783	-2.474917	-5.201856
1	-1.508363	-3.213463	-4.564060
1	-1.754086	-2.007235	-5.859309
1	-0.271451	-2.977925	-5.849236
1	-0.498840	1.952891	-1.964688
1	-0.333166	-0.418743	-1.246221

$(Ag_2O)_2$

47	-1.555813	0.554290	0.775981
47	0.160675	1.672658	-1.426262
8	-3.342753	1.930838	0.343175
47	-2.906684	1.644765	-1.682590
47	-1.547827	3.368037	0.383785
8	0.254373	1.965330	0.640922

O_2

8	-2.217341	-0.935114	-0.029227
8	-3.409525	-0.935114	-0.029227

$(Ag_2O)_2$-O_2

47	-3.411026	1.185302	1.384306
47	-2.789959	0.322889	-1.327308
8	-4.389882	1.281513	-0.398647
47	-0.996386	2.477153	2.446666
47	-1.280074	-0.541148	2.313229
8	-2.410280	1.061333	3.226642
8	-0.059467	0.510996	-0.439641
8	0.165774	1.649561	-0.160146

1-OIM1

47	-3.572796	1.594366	1.184784
47	-3.659035	-0.108143	-1.165929
8	-4.425119	-0.210719	0.733719
47	-1.133030	2.568529	0.138862
47	-1.692114	2.579532	3.229352
8	-2.565717	3.436331	1.477371
8	-0.016708	0.270291	2.464596
8	0.763929	0.840284	1.763902
6	-1.929642	-0.085606	-3.914758
6	-0.708816	-1.207155	-2.122221
6	-0.557695	-0.147804	-1.083909
1	-1.562444	-1.846611	-1.829097
8	-0.348051	1.025893	-1.338996
1	-0.639501	-0.510518	-0.033398
6	-1.896449	0.410183	-5.319519
1	-2.789833	0.045147	-5.846647
1	-1.955719	1.509335	-5.301143
1	-0.993777	0.105966	-5.864668
1	0.173531	-1.864815	-2.043395
7	-0.836772	-0.718849	-3.464844
8	-2.945244	0.099149	-3.220473
1	-0.038766	-0.795887	-4.090461

1-OTS1''

47	-3.537340	1.999002	1.231264
47	-3.781377	0.404648	-1.232847
8	-4.844826	0.611560	0.501072
47	-0.792277	2.561645	0.529520
47	-1.617729	1.763062	3.379756
8	-2.142603	3.385227	1.978072
8	-0.212466	-0.389061	1.263520
8	0.176764	0.774066	1.766403
6	-1.937208	-0.099680	-3.923699
6	-0.722707	-1.084945	-2.044170
6	-0.390847	0.078082	-1.166541
1	-1.647532	-1.507758	-1.607319
8	-0.279059	1.236867	-1.298974
1	-0.039162	-0.414671	0.205881
6	-1.927394	0.172733	-5.386777
1	-1.024696	-0.194477	-5.891200
1	-2.815945	-0.297958	-5.833525
1	-2.022195	1.258041	-5.541252
1	0.058521	-1.844367	-1.893495
7	-0.860950	-0.743293	-3.419533
8	-2.897814	0.244825	-3.226648
1	-0.070925	-0.924650	-4.036382

1-OIM2''

47	-1.682762	0.182676	1.112132
47	-1.564145	-1.041297	-1.438753
8	-2.690205	-1.380976	0.253029
47	-0.314686	1.946850	-0.577746

47	1.165627	0.497916	1.498016
8	-0.448961	1.823576	1.646142
8	2.019376	-1.869988	0.142501
8	2.670805	-1.004481	1.082473
6	0.418329	-1.257033	-3.972890
6	1.352113	-2.511168	-2.079834
6	1.940431	-1.432505	-1.228816
1	0.350374	-2.743952	-1.665923
8	2.248059	-0.323383	-1.481498
1	2.262179	-2.812946	0.311953
6	0.565394	-0.937640	-5.420039
1	1.384855	-1.484141	-5.904371
1	-0.383175	-1.166380	-5.928249
1	0.735942	0.144715	-5.521730
1	1.945897	-3.430575	-1.957099
7	1.295952	-2.138093	-3.458167
8	-0.478497	-0.716754	-3.307322
1	2.025865	-2.493046	-4.071323

1-OIM3’’

47	-3.432760	-0.528437	2.282110
47	-3.812075	0.772633	-0.361850
8	-4.950557	-0.334688	0.928796
47	-2.479119	1.189601	4.430939
47	-0.540150	0.072190	2.396491
8	-1.931176	-0.776352	3.743701
6	-1.140502	1.589983	-1.851978
6	-0.655376	1.567173	-0.433324
1	-0.936419	0.608985	-2.304829
8	-1.219297	1.964073	0.547584
8	0.578791	0.986781	-0.413019
8	1.069836	0.804370	0.887962
1	1.452824	1.675052	1.125955
1	-0.531506	2.332929	-2.398914
7	-2.561207	1.876705	-1.951457
6	-2.954310	3.224414	-1.870302
8	-2.203651	4.058374	-1.407726
6	-4.313470	3.524439	-2.405265
1	-4.197083	3.870186	-3.446043
1	-4.977561	2.648670	-2.405234
1	-4.760717	4.344795	-1.828727
1	-3.009962	1.377528	-2.725208

1-OTS2’’

47	-3.615947	0.162946	2.280195
47	-3.915317	0.558871	-0.565965
8	-4.992318	1.095555	1.093347
47	-1.834234	1.080597	4.419419
47	-0.784086	-0.168845	1.921883
8	-2.117859	-0.805858	3.419360
6	-0.656559	1.884550	-0.950636
8	-0.499193	2.687519	-0.000972
8	-0.100915	0.715596	-0.827068
8	0.574885	0.687652	0.422871
1	0.133906	2.035225	0.608997
6	-1.432841	2.194281	-2.173952
1	-2.474039	2.379483	-1.845918
1	-1.065934	3.160636	-2.552231
7	-1.360180	1.195512	-3.195580
6	-2.104210	0.073909	-3.222738
8	-2.952829	-0.204109	-2.363789
6	-1.867879	-0.857526	-4.360682
1	-2.820051	-1.015124	-4.888700
1	-1.109447	-0.496851	-5.066938
1	-1.557284	-1.831507	-3.953537
1	-0.660093	1.316111	-3.924141

1-OTS1’

47	-2.909352	2.263337	-0.323209
47	-2.520175	-0.364540	-1.839718
8	-3.989727	0.649636	-0.829132
47	-0.570203	3.596918	-1.610487
47	-0.650928	2.623586	1.259022
8	-1.818843	3.965016	0.170376
8	0.423101	0.969062	1.993547
8	0.403966	-0.058869	1.262044
6	0.067799	-1.208766	-3.457510
6	1.078945	-0.751350	-1.259029
6	0.403338	0.513275	-0.785259
1	0.543252	-1.624776	-0.855288
8	0.925785	1.618655	-0.856243

1	-0.707211	0.417574	-0.607672
6	0.291285	-1.310190	-4.926745
1	0.026500	-2.328206	-5.249669
1	-0.399803	-0.620095	-5.434343
1	1.322317	-1.085037	-5.227413
1	2.115670	-0.767703	-0.895271
7	1.104095	-0.813441	-2.707083
8	-1.039462	-1.508299	-2.969648
1	1.971350	-0.574240	-3.181979

1-OIM2'

47	-2.904793	2.279263	-0.455579
47	-2.407826	-0.441349	-1.716096
8	-3.887398	0.563566	-0.767504
47	-0.487364	3.247830	-1.847486
47	-0.549041	2.707586	1.038511
8	-1.739893	3.964343	-0.140371
8	0.559674	1.032267	1.760398
8	0.305984	0.011374	0.918122
6	0.050244	-1.180971	-3.366028
6	1.056687	-0.867317	-1.151489
6	0.390413	0.357404	-0.470838
1	0.524733	-1.774290	-0.826973
8	0.860887	1.510941	-0.756811
1	-0.757677	0.231336	-0.758765
6	0.245937	-1.094283	-4.837925
1	0.075763	-2.091574	-5.270750
1	-0.523065	-0.425656	-5.253903
1	1.242109	-0.732672	-5.122469
1	2.095244	-0.910761	-0.793706
7	1.057853	-0.774448	-2.581393
8	-1.013343	-1.638602	-2.896135
1	1.876571	-0.372440	-3.033521

1-OTS1

47	-2.879500	2.252508	-0.324796
47	-2.314130	-0.433517	-1.640914
8	-3.739311	0.441203	-0.554615
47	-0.644754	3.507117	-1.808417
47	-0.523724	2.826225	1.049147
8	-1.856204	4.048024	-0.060642
8	0.577003	1.104030	1.713594
8	0.312190	0.070348	0.876287
6	0.054207	-1.167091	-3.427601
6	0.960540	-0.931932	-1.162043
6	0.438861	0.363923	-0.486396
1	0.333383	-1.782558	-0.858475
8	0.855964	1.479604	-0.857949
1	-0.864272	0.236405	-0.760108
6	0.344111	-1.119669	-4.884545
1	0.129074	-2.110134	-5.313189
1	-0.346271	-0.405131	-5.357495
1	1.380597	-0.837923	-5.108569
1	1.974449	-1.082257	-0.761634
7	1.041677	-0.837023	-2.586504
8	-1.072008	-1.528749	-3.024399
1	1.909816	-0.491858	-2.991448

1-OIM2

47	-3.197821	2.079520	0.169539
47	-2.618790	-0.076747	-1.592705
8	-4.189380	0.399713	-0.359786
47	-0.869457	3.278970	-1.058140
47	-0.648666	2.607252	1.701889
8	-2.142341	3.757578	0.736478
8	0.950385	1.263952	2.115307
8	0.681197	0.069286	1.397410
6	0.126434	-0.989252	-2.981705
6	0.348350	-1.176437	-0.525603
6	0.682034	0.169654	0.076721
1	-0.748840	-1.302973	-0.478412
8	0.879774	1.182131	-0.563807
1	-2.064567	1.587952	-1.007182
6	0.840664	-1.142125	-4.280919
1	0.272697	-1.838154	-4.916097
1	0.846289	-0.167367	-4.791442
1	1.871184	-1.502661	-4.169744
1	0.772098	-1.975741	0.098282
7	0.811730	-1.309624	-1.877370
8	-1.055273	-0.595498	-2.989893
1	1.784650	-1.578453	-2.005908

1-OTS2

47	-3.044082	2.093119	0.122448
47	-2.571015	0.073566	-1.878270
8	-4.197978	0.811922	-0.943371
47	-1.437273	4.645317	-0.214775
47	-0.526578	2.581852	1.723217
8	-2.341942	3.578696	1.418098
8	1.314032	1.469538	1.696226
8	1.127356	0.216144	1.083851
6	0.166790	-1.150718	-3.028287
6	0.265648	-1.216468	-0.547539
6	0.427542	0.178487	-0.014163
1	-0.816241	-1.442519	-0.555375
8	-0.069012	1.177981	-0.555083
1	-1.557148	1.217502	-0.694040
6	0.935329	-1.406320	-4.279555
1	0.403923	-2.171231	-4.865500
1	0.942324	-0.484442	-4.880049
1	1.966359	-1.735314	-4.098113
1	0.750531	-1.933699	0.126577
7	0.816006	-1.355311	-1.873418
8	-1.017218	-0.780694	-3.110534
1	1.794998	-1.626427	-1.935431

1-OIM3

47	-3.441124	-0.626127	2.294190
47	-3.783138	0.923046	-0.239646
8	-4.980896	-0.053908	1.087055
47	-2.323109	0.477476	4.755938
47	-0.554229	-0.206946	2.430011
8	-1.909063	-1.287037	3.593402
6	-1.126454	1.714694	-1.835950
6	-0.585421	1.718376	-0.455393
1	-0.869176	0.749730	-2.291758
8	-0.913167	2.571357	0.421726
8	0.278126	0.815295	-0.165239
8	0.755892	0.971109	1.161669
1	-0.578108	2.503530	-2.385190
7	-2.566240	1.921939	-1.907656
6	-3.021120	3.257638	-1.977187
8	-2.305840	4.165815	-1.615172
6	-4.390368	3.426762	-2.539431
1	-4.300887	3.478407	-3.637676
1	-5.054473	2.585511	-2.293776
1	-4.818892	4.372351	-2.184563
1	-2.996272	1.322953	-2.620058
1	-0.338803	2.326638	1.219819

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47	-3.351204	1.216216	1.497668
47	-3.719982	0.225910	-1.272269
8	-4.827578	1.266732	0.131903
47	-0.820806	2.811485	0.687967
47	-1.205858	-0.217065	0.258202
8	-1.748314	1.113185	2.827825
8	-0.533158	1.059350	1.980262

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6	-0.267741	-0.213586	-2.263171
6	-0.982992	1.080722	-2.546572
1	-1.361298	-1.970561	-2.731634
1	0.814013	-0.027042	-2.371118
8	-1.916608	1.216774	-3.301179
7	-0.694457	-1.296543	-3.095425
6	-0.376582	-1.321686	-4.411007
8	0.352987	-0.467953	-4.913711
6	-0.959286	-2.443152	-5.211268
1	-1.469361	-3.198999	-4.598857
1	-1.677959	-2.022424	-5.931902
1	-0.157532	-2.918791	-5.794910
1	-0.430304	-0.462750	-1.203476
8	-0.454066	2.077316	-1.839938
1	-0.949325	2.894226	-2.034587

1-OIM4

47	-4.233922	1.853733	1.076164
47	-3.388974	0.183504	-1.132828
8	-5.129489	1.093469	-0.577374
47	-1.040940	1.695678	0.707105
47	-2.682021	-0.486478	1.683446
8	-3.066161	2.361906	2.735322
8	-1.915022	1.441910	2.666633

6	-1.233403	-0.266293	-3.116514
6	1.083687	-0.289452	-2.423286
6	0.966745	0.639253	-1.264998
1	1.094240	-1.312288	-2.002284
8	0.141841	1.534412	-1.193732
1	1.685925	0.450172	-0.437220
6	-2.229814	0.104167	-4.157654
1	-3.033234	-0.647072	-4.175413
1	-2.684344	1.067418	-3.869615
1	-1.785937	0.208428	-5.156736
1	2.080954	-0.154377	-2.871660
7	0.062037	-0.121939	-3.416859
8	-1.572276	-0.682960	-1.987392
1	0.313961	0.227100	-4.338386

1-OTS3

47	-2.934267	2.318178	-0.349794
47	-2.406615	-0.658115	-1.303766
8	-3.708492	0.426520	-0.319003
47	-0.523594	3.158445	-1.833491
47	-0.460841	2.855621	1.021672
8	-1.786320	4.050674	-0.268555
8	0.239405	0.735335	0.822364
6	0.012943	-1.960202	-2.800209
6	0.844103	-1.123212	-0.639383
6	0.402324	0.360501	-0.516327
1	0.153092	-1.767258	-0.077511
8	0.687808	1.148809	-1.446352
1	-0.908909	0.109855	-0.601057
6	0.383390	-2.401968	-4.171514
1	-0.053619	-3.395302	-4.350886
1	-0.073456	-1.710576	-4.896146
1	1.468185	-2.439124	-4.333155
1	1.824982	-1.167238	-0.142204
7	1.003399	-1.575290	-1.989057
8	-1.188094	-1.984177	-2.452920
1	1.933020	-1.513006	-2.399409

1-OIM5

47	-3.354729	1.410599	1.352819
47	-3.621929	-0.118849	-1.055082
8	-4.648851	-0.011173	0.723813
47	-0.808006	2.123307	0.292808
47	-0.865175	1.401954	3.203414
8	-1.945286	2.808442	1.975380
6	-1.803547	-0.277334	-3.771729
6	-0.519923	-1.408213	-2.024700
6	-0.219554	-0.370430	-0.949807
1	-1.429987	-1.942677	-1.701617
8	-0.076608	0.837707	-1.323961
6	-1.797167	0.276183	-5.156166
1	-2.691617	-0.079899	-5.687716
1	-1.871809	1.372905	-5.091962
1	-0.897108	0.008166	-5.724449
1	0.289671	-2.152529	-2.027084
7	-0.698169	-0.899215	-3.357395
8	-2.830347	-0.151397	-3.073553
1	0.102465	-0.892918	-3.984261
8	-0.177161	-0.790333	0.216318
1	-2.648115	1.191894	-0.180237

1-OTS4

47	-2.968791	2.554373	-0.578462
47	-2.313854	0.304680	-2.265374
8	-3.545392	1.943685	-2.403545
47	-0.929366	4.490050	0.619361
47	-1.368484	1.687476	1.682844
8	-2.622600	3.352984	1.312703
8	-0.111713	-0.045973	1.242395
6	0.088362	-1.406375	-2.661548
6	1.034986	-1.212375	-0.442252
6	0.259688	0.004989	0.038552
1	0.539742	-2.101834	-0.019742
8	0.040756	0.952245	-0.757955
1	-1.575119	1.507572	-0.746952
6	0.301356	-1.391494	-4.134701
1	-0.187620	-2.273301	-4.574966
1	-0.199030	-0.501076	-4.548073
1	1.361817	-1.375825	-4.416959
1	2.040541	-1.174595	0.000717
7	1.158899	-1.317344	-1.871715

8	-1.061256	-1.501746	-2.170974
1	2.075398	-1.224673	-2.302670

1-OIM6

47	-3.395380	2.116426	1.111699
47	-3.552839	0.800290	-1.475864
8	-4.563747	2.325934	-0.550080
47	-0.941412	0.669936	1.528963
47	-3.325609	0.166112	3.306001
8	-2.127044	1.873109	2.792616
6	-1.780455	-0.640104	-3.473803
6	0.316286	-1.069688	-2.374594
6	0.022679	-0.109649	-1.254932
1	0.146012	-2.084451	-1.982335
8	-0.206757	1.121449	-1.643512
6	-2.524297	-0.245047	-4.697688
1	-3.449359	-0.835452	-4.765753
1	-2.813957	0.813865	-4.594783
1	-1.931002	-0.363989	-5.613900
1	1.386446	-0.986646	-2.617032
7	-0.456267	-0.803892	-3.559177
8	-2.342270	-0.792845	-2.367573
1	0.011123	-0.683905	-4.454405
8	0.042389	-0.471999	-0.085151
1	-0.441310	1.691188	-0.881774

2-OIM1

47	-3.156964	2.865125	1.094296
47	-3.545930	1.089049	-1.119210
8	-4.715980	1.689488	0.489570
47	-0.550069	2.527313	0.071626
47	-1.038089	2.322905	3.015744
8	-1.333542	3.866159	1.536545
8	-2.170614	-0.631284	1.770315
8	-2.180246	-0.099593	2.839223
6	-1.848045	0.125768	-3.892402
6	-0.639364	-1.244229	-2.205913
6	-0.345095	-0.206740	-1.173316
8	-0.084457	0.954307	-1.434106
1	-0.341212	-0.579087	-0.123585
6	-1.971692	0.383947	-5.357685
1	-2.739146	-0.301964	-5.753378
1	-2.319822	1.411954	-5.523519
1	-1.036079	0.207113	-5.904809
1	0.310473	-1.814251	-2.257962
7	-0.853167	-0.701485	-3.526550
8	-2.649988	0.634963	-3.099029
1	-0.294498	-1.104141	-4.274967
6	-1.666070	-2.266847	-1.686940
6	-2.036615	-3.289673	-2.759971
1	-1.163466	-2.798106	-0.859960
6	-2.564429	-4.577592	-2.137912
6	-3.040941	-5.574867	-3.177586
1	-3.241400	-6.538693	-2.670109
1	-2.225399	-5.747159	-3.907319
8	-2.831243	-1.685743	-1.155484
1	-3.442146	-1.569137	-1.905566
8	-4.205180	-5.073066	-3.802963
1	-4.368193	-5.576557	-4.612482
1	-1.117171	-3.557736	-3.326693
1	-3.422177	-4.314327	-1.481911
8	-2.996647	-2.685825	-3.598150
1	-3.607797	-3.382890	-3.911368
8	-1.501538	-5.140359	-1.405729
1	-1.849238	-5.878363	-0.885911

2-OTS1

47	-2.511546	2.388541	0.077890
47	-2.465681	-0.129242	-1.547738
8	-3.626472	0.714691	-0.152515
47	-0.347638	3.293717	-1.659461
47	0.073778	2.450050	1.116584
8	-1.165494	3.968711	0.280810
8	0.972042	0.527876	1.512305
8	0.495037	-0.394733	0.632074
6	-0.382765	-0.767188	-3.755847
6	0.780393	-1.248493	-1.592857
6	0.497783	0.000252	-0.698156
8	0.994271	1.092843	-1.033606
1	-0.871591	0.094504	-0.799772
6	-0.167746	-0.388699	-5.179721

1	-0.747404	-1.070613	-5.818320	1	0.306143	-1.005049	-5.344456
1	-0.573191	0.624178	-5.330840	1	1.238894	0.385164	-4.767903
1	0.888348	-0.404415	-5.477589	1	1.859888	-1.273637	-4.485815
1	1.854758	-1.416545	-1.408760	1	0.724152	-2.291781	-0.439050
7	0.709669	-0.890179	-2.990187	7	0.679831	-1.348843	-2.239814
8	-1.540661	-0.958821	-3.332822	8	-0.904819	-0.027999	-3.215773
1	1.593849	-0.638433	-3.426659	1	1.579728	-1.792988	-2.402053
6	0.084713	-2.571226	-1.223740	6	-1.337553	-1.881001	-0.817178
6	0.954637	-3.388373	-0.259760	6	-1.530245	-3.049018	0.152352
1	0.067222	-3.166495	-2.163666	1	-1.631500	-2.262975	-1.818110
6	0.289976	-4.706617	0.121634	6	-2.987007	-3.487288	0.244512
1	1.119402	-2.808094	0.671213	1	-1.198175	-2.730440	1.162653
6	1.205353	-5.631127	0.886378	6	-3.173418	-4.710036	1.110478
1	-0.026620	-5.224136	-0.811332	1	-3.341059	-3.726523	-0.783038
1	2.084181	-5.887493	0.266422	1	-2.620552	-5.565727	0.680324
1	1.568909	-5.103673	1.792017	1	-2.752345	-4.501431	2.114790
8	-1.216388	-2.379274	-0.735548	8	-2.111750	-0.764966	-0.452071
1	-1.416641	-3.088925	-0.090591	1	-2.946706	-1.084153	-0.050929
8	2.168184	-3.634973	-0.932764	8	-0.745368	-4.111556	-0.338271
1	2.882669	-3.685852	-0.283580	1	-0.437626	-4.644894	0.406837
8	-0.840010	-4.398935	0.920861	8	-3.739215	-2.416439	0.786918
1	-1.233927	-5.239640	1.201893	1	-4.634244	-2.753448	0.952425
8	0.442325	-6.769323	1.215144	8	-4.560402	-4.953840	1.168987
1	0.939106	-7.300432	1.850511	1	-4.735912	-5.561487	1.898933

2-OIM2

47	-2.977625	3.086582	-0.151480
47	-2.435482	1.153934	-2.176934
8	-4.055209	2.349363	-1.677399
47	-0.399934	4.678165	0.213871
47	-0.792297	2.167907	1.729117
8	-1.984862	3.880590	1.467043
8	0.523923	0.550214	2.110374
8	0.320329	-0.527422	1.214300
6	0.170311	-0.645449	-3.261522
6	0.148655	-1.474633	-0.900110
6	0.427604	-0.229878	-0.072080
8	0.703917	0.859608	-0.522985
1	-1.754058	2.174512	-0.840389
6	0.956759	-0.651912	-4.530574

2-OTS2

47	-2.889131	2.510987	0.710830
47	-2.836980	0.745534	-1.525800
8	-4.295657	1.460062	-0.334343
47	-1.276210	4.993509	0.346223
47	-0.084869	2.660334	1.784677
8	-1.835919	3.766153	2.023121
8	1.669500	1.524514	1.333668
8	1.351578	0.276445	0.772835
6	-0.603082	-0.928612	-3.029641
6	0.189069	-1.185009	-0.573566
6	0.446064	0.249200	-0.170637
8	-0.109328	1.263074	-0.606402
1	-1.576180	1.491525	-0.458217
6	-0.391692	-1.602750	-4.345718

1	-1.250571	-2.277878	-4.504037
1	-0.412493	-0.850536	-5.145956
1	0.535032	-2.188286	-4.399751
1	1.105251	-1.720553	-0.285795
7	0.126285	-1.414176	-2.014251
8	-1.445617	-0.017604	-2.963852
1	0.711675	-2.202275	-2.282275
6	-0.896208	-1.789383	0.366758
6	-1.504388	-3.086228	-0.163108
1	-0.317076	-2.054390	1.272451
6	-2.611986	-2.843196	-1.193032
1	-2.006064	-3.578122	0.695234
6	-2.924044	-4.047060	-2.040152
1	-2.341785	-2.025071	-1.886199
1	-2.002009	-4.363221	-2.564599
1	-3.249778	-4.883903	-1.388214
8	-1.870774	-0.851770	0.745812
1	-2.752157	-1.157648	0.450048
8	-0.443577	-3.876645	-0.638583
1	-0.700698	-4.807461	-0.590415
8	-3.745984	-2.432585	-0.439773
1	-4.434207	-2.162024	-1.066570
8	-3.932799	-3.657178	-2.943116
1	-4.207022	-4.431786	-3.450926

8	-2.005014	4.201280	-1.800164
6	-4.269961	3.619055	-2.299344
1	-4.754392	2.801095	-2.851866
1	-4.812016	3.755876	-1.348880
1	-4.339452	4.558512	-2.863695
1	-3.011849	1.391728	-2.579381
1	-0.455780	2.386794	1.202414
6	-0.801745	0.254097	-2.509834
6	-1.458330	0.124186	-3.889047
1	-1.249644	-0.542843	-1.873151
6	-0.870119	-1.037247	-4.683262
1	-1.271210	1.051671	-4.471872
6	-1.684100	-1.400296	-5.902174
1	-0.808117	-1.931211	-4.024468
1	-2.684858	-1.758330	-5.596645
1	-1.820831	-0.492564	-6.524834
8	0.591912	0.115390	-2.558918
1	0.858163	-0.131340	-3.467584
8	-2.843131	-0.062723	-3.669399
1	-3.330916	0.173178	-4.473242
8	0.425481	-0.632527	-5.089238
1	0.783314	-1.339609	-5.649683
8	-0.955966	-2.395646	-6.582721
1	-1.322950	-2.493860	-7.470849

2-OIM3

47	-3.580580	-0.650297	2.215517
47	-3.789165	0.930870	-0.302132
8	-5.057244	-0.087672	0.927511
47	-2.596495	0.460915	4.750141
47	-0.726855	-0.147370	2.508816
8	-2.105644	-1.283531	3.590321
6	-1.093689	1.617243	-1.855147
6	-0.585925	1.686811	-0.446446
8	-0.977955	2.587423	0.353793
8	0.260386	0.818073	-0.031754
8	0.620993	1.064680	1.319910
1	-0.503269	2.379476	-2.406974
7	-2.509907	1.974897	-1.884816
6	-2.838127	3.340874	-1.987304

2-OIM4

47	-3.677558	1.743185	1.534059
47	-3.424251	0.458389	-1.053202
8	-4.868873	1.534745	-0.096551
47	-0.677837	1.345986	0.620455
47	-2.417608	-0.842283	1.420026
8	-2.261436	1.710317	3.071419
8	-1.261818	0.722358	2.617536
6	-1.532519	-0.123202	-3.297990
6	0.851680	-0.479316	-2.807629
6	0.990981	0.488796	-1.670964
8	0.229900	1.418640	-1.468952
1	1.864746	0.302650	-1.006487
6	-2.517299	0.475295	-4.240176
1	-3.420278	-0.152227	-4.268128

1	-2.812434	1.459877	-3.839148
1	-2.118545	0.611120	-5.254051
1	1.766844	-0.362582	-3.414129
7	-0.251728	-0.164413	-3.685090
8	-1.873839	-0.564556	-2.181871
1	-0.025534	0.214889	-4.601225
6	0.883043	-1.913161	-2.231596
6	2.300158	-2.484872	-2.305932
1	0.255234	-2.543144	-2.898065
6	2.388930	-3.881059	-1.700450
1	2.982625	-1.821707	-1.730674
6	3.725609	-4.542494	-1.935924
1	1.598505	-4.514186	-2.162086
1	3.893242	-4.682632	-3.019912
1	4.525389	-3.878863	-1.549420
8	0.382177	-1.906394	-0.914998
1	0.826839	-2.618525	-0.411749
8	2.646041	-2.519842	-3.670395
1	3.605053	-2.428367	-3.754606
8	2.171674	-3.760107	-0.305942
1	2.347866	-4.631387	0.084303
8	3.689620	-5.770340	-1.244625
1	4.593515	-6.094102	-1.140286

2-OTS3

47	-2.597419	2.447598	-0.464010
47	-2.380052	-0.315933	-2.021488
8	-3.674573	0.836119	-1.087011
47	0.179623	3.009684	-1.250927
47	-0.409875	2.104474	1.416413
8	-1.207232	3.799594	0.269201
8	0.006819	-0.022696	0.819581
6	0.070215	-1.741443	-3.344442
6	0.662995	-1.624386	-0.901638
6	0.321621	-0.130937	-0.477876
8	0.907853	0.759935	-1.151192
1	-0.939831	-0.231634	-0.985399
6	0.655860	-1.917625	-4.703159
1	0.143052	-2.756374	-5.196831
1	0.440602	-1.013888	-5.293547
1	1.737803	-2.101237	-4.693296
1	1.655399	-1.745419	-0.433861
7	0.923559	-1.756226	-2.312880
8	-1.166480	-1.605751	-3.234773
1	1.908094	-1.795690	-2.566979
6	-0.247674	-2.702645	-0.285846
6	0.301136	-3.106962	1.089835
1	-0.120878	-3.602408	-0.920778
6	-0.759222	-3.743786	1.976873
1	0.648513	-2.202758	1.628235
6	-0.177884	-4.398153	3.204616
1	-1.320839	-4.511943	1.401529
1	0.485855	-5.230302	2.903547
1	0.438835	-3.652867	3.748085
8	-1.612895	-2.378771	-0.284183
1	-1.885072	-2.160734	0.629242
8	1.381276	-3.975390	0.832553
1	2.016642	-3.903087	1.557665
8	-1.624006	-2.685794	2.362328
1	-2.279308	-3.055969	2.973774
8	-1.263428	-4.844828	3.983866
1	-0.931763	-5.097947	4.854875

2-OIM5

47	-3.424243	1.546538	1.396813
47	-3.819916	0.671178	-1.283531
8	-5.074192	1.232289	0.283008
47	-0.665856	1.347975	0.683019
47	-1.650194	-0.312003	3.018089
8	-1.680390	1.793881	2.509153
6	-1.821100	0.112052	-3.927259
6	-0.696657	-1.522248	-2.392228
6	-0.216606	-0.712819	-1.183451
8	-0.169721	0.550922	-1.302737
6	-1.677517	0.826792	-5.231957
1	-2.581210	0.647159	-5.833352
1	-1.631849	1.908186	-5.031159
1	-0.790221	0.526334	-5.804156
1	0.103304	-2.246009	-2.615385
7	-0.850136	-0.753609	-3.612391

8	-2.824187	0.327991	-3.225847
1	-0.075965	-0.809123	-4.268764
8	0.064409	-1.352292	-0.157422
1	-2.560810	1.190428	-0.036851
6	-1.932006	-2.359478	-1.994331
6	-1.488301	-3.735993	-1.488585
1	-2.505361	-2.556872	-2.923067
6	-2.581078	-4.457863	-0.711146
1	-0.639333	-3.606336	-0.788791
6	-2.262611	-5.911570	-0.467163
1	-3.541261	-4.396858	-1.269250
1	-2.193269	-6.444944	-1.433585
1	-1.273177	-5.981050	0.030121
8	-2.769993	-1.683361	-1.085400
1	-2.818974	-2.187066	-0.247946
8	-1.090988	-4.459466	-2.630903
1	-0.418856	-5.104379	-2.371151
8	-2.693457	-3.781168	0.533453
1	-3.350492	-4.257776	1.064672
8	-3.292303	-6.424448	0.346260
1	-3.018883	-7.288648	0.679784

2-OTS4

47	-2.798031	1.348945	0.853737
47	-2.446801	-0.470055	-1.377644
8	-4.043765	0.418690	-0.416172
47	-1.043034	3.841188	1.003453
47	-0.107974	1.179430	2.042804
8	-1.820660	2.384270	2.380485
8	1.147718	-0.184828	0.861007
6	-0.009664	-1.223736	-3.351403
6	1.182861	-1.399022	-1.157855
6	0.755102	-0.189209	-0.333509
8	0.012189	0.681179	-0.864745
1	-1.473012	0.786671	-0.204265
6	0.185791	-1.006848	-4.815774
1	-0.258961	-1.854707	-5.357978
1	-0.372957	-0.105538	-5.110928
1	1.237913	-0.895388	-5.108172
1	2.251870	-1.563071	-0.956209
7	1.092352	-1.209517	-2.591371
8	-1.153318	-1.429166	-2.906904
1	1.968626	-1.021044	-3.070746
6	0.432428	-2.641003	-0.618047
6	1.313978	-3.386230	0.386541
1	0.300461	-3.340043	-1.470968
6	0.560738	-4.485763	1.124064
1	1.679169	-2.670326	1.151061
6	1.471740	-5.384179	1.923728
1	0.011147	-5.109507	0.384319
1	2.167666	-5.912101	1.245657
1	2.076095	-4.757069	2.610815
8	-0.821247	-2.280019	-0.087653
1	-0.959676	-2.750416	0.759893
8	2.382996	-3.920611	-0.359940
1	3.159998	-3.983371	0.211534
8	-0.351875	-3.842016	1.998911
1	-0.780747	-4.533448	2.527510
8	0.642335	-6.278554	2.629141
1	1.170785	-6.718575	3.307439

2-OIM6

47	-3.841703	2.457935	0.933161
47	-3.638723	1.092332	-1.563817
8	-4.869285	2.570353	-0.836578
47	-1.428842	0.988287	1.469307
47	-3.864908	0.538941	3.162498
8	-2.645648	2.237583	2.667129
6	-1.687148	-0.637812	-3.225296
6	0.429941	-1.090562	-2.093961
6	0.026797	-0.048809	-1.057499
8	0.124622	1.169515	-1.543784
6	-2.430779	-0.494626	-4.503596
1	-3.380286	-1.044696	-4.429819
1	-2.676570	0.571549	-4.638149
1	-1.858341	-0.842215	-5.373312
1	1.473442	-0.838706	-2.363164
7	-0.378668	-0.902522	-3.282271
8	-2.235942	-0.478254	-2.115175
1	0.021619	-1.237597	-4.155916

8	-0.292815	-0.299694	0.093060
1	-0.149243	1.830598	-0.877518
6	0.421474	-2.527329	-1.570072
6	1.069599	-3.519718	-2.551261
1	-0.637279	-2.820160	-1.386286
6	0.746872	-4.960271	-2.163905
1	2.163499	-3.353651	-2.455355
6	1.554469	-5.965669	-2.949547
1	-0.332086	-5.122402	-2.383459
1	1.342459	-5.861324	-4.030696
1	2.631489	-5.756762	-2.791511
8	1.178474	-2.539701	-0.383881
1	1.260623	-3.475983	-0.125688
8	0.651806	-3.299365	-3.879933
1	1.352504	-3.595989	-4.476082
8	0.994387	-5.144444	-0.783955
1	1.018509	-6.102339	-0.628257
8	1.199111	-7.240129	-2.462816
1	1.870190	-7.875774	-2.743137

NAGA

6	-3.664995	-0.473246	0.631339
6	-2.486869	-0.120895	-0.241364
6	-1.341530	-1.116361	-0.119693
6	-0.015625	-0.628255	-0.716321
6	-0.036714	-0.154212	-2.188553
6	-0.708653	1.186853	-2.448335
8	-1.985331	1.151501	0.121051
8	-4.643211	0.516983	0.414546
8	-1.666507	-2.342109	-0.740063
1	-5.317026	0.440620	1.102445
1	-1.177034	-1.886402	-2.623505
1	-4.037940	-1.484423	0.373403
1	-1.127307	-1.268406	0.959206
1	1.025278	0.017553	-2.443840
1	-3.331259	-0.496022	1.687943
8	0.595239	0.321476	0.115192
1	0.635409	-1.521338	-0.724840
1	-2.401282	-2.758580	-0.268824
1	-0.081421	0.991079	0.317664

1	-2.831878	-0.109838	-1.297241
8	-1.771863	1.340123	-3.003538
7	-0.574390	-1.177597	-3.043286
6	-0.414520	-1.109204	-4.383561
8	0.246647	-0.213830	-4.909825
6	-1.096463	-2.173510	-5.183387
1	-1.479659	-2.999021	-4.568509
1	-1.937810	-1.715791	-5.727457
1	-0.396063	-2.562605	-5.936340
1	-2.741053	1.756379	0.182117
8	0.049243	2.197646	-2.034005
1	-0.425506	3.031695	-2.208947

2-IM1

6	-3.734812	-0.793983	0.630604
6	-2.687901	-0.186291	-0.269201
6	-1.326929	-0.853853	-0.115966
6	-0.164680	-0.052442	-0.711796
6	-0.263292	0.345808	-2.204636
6	-1.060728	1.611629	-2.448203
8	-2.525238	1.183973	0.049393
8	-4.912863	-0.046844	0.437250
8	-1.302756	-2.127615	-0.714000
1	-5.516267	-0.225185	1.170288
1	-1.069861	-1.576630	-2.593041
1	-3.872805	-1.864412	0.380470
1	-1.096931	-0.923152	0.968306
1	0.761772	0.663723	-2.481504
1	-3.381127	-0.733772	1.678736
8	0.091808	1.092329	0.089573
1	0.713918	-0.715649	-0.645445
1	-1.902521	-2.721265	-0.240924
1	-0.772616	1.363857	0.474695
1	-3.026899	-0.293109	-1.321699
8	-0.632595	2.703109	-2.078376
7	-0.640690	-0.760245	-3.031972
6	-0.440863	-0.695527	-4.371262
8	0.057154	0.301007	-4.891497
6	-0.881256	-1.883005	-5.163830
1	-1.129555	-2.753267	-4.541608

1	-1.769542	-1.599968	-5.750463
1	-0.090458	-2.148511	-5.879990
1	-3.406126	1.544908	0.243877
12	0.809372	2.955182	-0.613914
8	2.651421	2.553537	-1.361588
1	3.354876	2.346911	-0.726887
8	0.483309	4.100441	0.827081
1	0.715950	5.031289	0.765615
1	2.745743	1.899939	-2.071765
8	-2.182572	1.477554	-3.093747
1	-2.598684	2.353634	-3.222201

2-TS1

6	-3.668700	-0.448944	0.611500
6	-2.564452	0.016768	-0.307063
6	-1.250991	-0.709184	-0.049968
6	-0.004887	-0.122338	-0.729419
6	-0.155874	0.281453	-2.216611
6	-0.877929	1.592286	-2.450337
8	-2.355263	1.399667	-0.137899
8	-4.824242	0.273947	0.256889
8	-1.345277	-2.047630	-0.497021
1	-5.489808	0.148072	0.945546
1	-1.132179	-1.575408	-2.512439
1	-3.823310	-1.541225	0.505480
1	-1.035751	-0.672764	1.039425
1	0.875451	0.520237	-2.546339
1	-3.365258	-0.250794	1.658907
8	0.596114	0.902629	-0.000648
1	0.692606	-0.981881	-0.766538
1	-2.057656	-2.496696	-0.021071
1	0.026882	1.541116	0.695317
1	-2.885336	-0.199463	-1.349570
8	-0.410984	2.664270	-2.068898
7	-0.656055	-0.813342	-2.997683
6	-0.484642	-0.840173	-4.341141
8	0.092290	0.071502	-4.931167
6	-1.054001	-2.024033	-5.054505
1	-1.384112	-2.822901	-4.377121
1	-1.913825	-1.688213	-5.655447
1	-0.302379	-2.415404	-5.755172
1	-3.227397	1.822438	-0.180690
12	0.906617	2.944821	-0.516250
8	2.658237	3.001602	-1.528694
1	3.502585	2.946506	-1.055495
8	-0.117850	2.823919	1.169559
1	-1.063466	2.995484	1.084170
1	2.740309	2.384024	-2.272708
8	-1.979156	1.524507	-3.145642
1	-2.347261	2.422010	-3.268440

2-IM2

6	-3.295073	-0.268014	0.837780
6	-2.157128	0.189488	-0.045659
6	-1.132729	-0.909123	-0.306569
6	0.112186	-0.495731	-1.117634
6	-0.180521	-0.023555	-2.578235
6	-0.908319	1.296718	-2.687648
8	-1.535100	1.299152	0.596049
8	-4.093613	0.868744	1.076545
8	-1.771265	-1.981986	-0.972176
1	-4.635484	0.711468	1.860821
1	-1.373942	-1.724609	-2.922754
1	-3.861099	-1.072597	0.333736
1	-0.737211	-1.238249	0.676302
1	0.822034	0.217690	-2.983773
1	-2.876180	-0.677304	1.778084
8	0.884286	0.408258	-0.444682
1	0.641176	-1.464692	-1.286243
1	-2.228437	-2.543912	-0.332415
1	-2.596098	0.517230	-1.014303
8	-0.628681	2.281660	-2.007783
7	-0.755669	-1.061324	-3.388883
6	-0.505693	-1.160257	-4.714225
8	0.230696	-0.368518	-5.301808
6	-1.191892	-2.284129	-5.425457
1	-1.661750	-3.007709	-4.745643
1	-1.966519	-1.860359	-6.084030
1	-0.464131	-2.797455	-6.070588
1	-2.256885	1.843110	0.963077

12 0.238919 2.199739 -0.105841
8 2.063109 3.122734 -0.368643
1 2.298228 3.929418 0.113189
8 -0.412405 3.940236 0.776406
1 -0.001628 4.780874 0.523949
1 2.864592 2.578982 -0.372032
1 -1.364075 4.117810 0.816892
8 -1.844230 1.340533 -3.603444
1 -2.232283 2.237388 -3.625468

2-TS2

6 -3.229732 -0.327012 0.797825
6 -2.052201 0.096841 -0.043714
6 -0.977140 -0.981046 -0.115864
6 0.379299 -0.558605 -0.628200
6 -0.031853 0.013492 -2.894983
6 -0.633677 1.264590 -2.719878
8 -1.526719 1.302486 0.514396
8 -4.118543 0.765623 0.815674
8 -1.425959 -2.056645 -0.901250
1 -4.711089 0.672508 1.573167
1 -1.151474 -1.755588 -3.006514
1 -3.686550 -1.234680 0.360553
1 -0.753702 -1.316958 0.922774
1 1.063579 0.019632 -2.941517
1 -2.873668 -0.579224 1.815626
8 0.976049 0.449179 -0.200226
1 0.947249 -1.407791 -1.060317
1 -1.911236 -2.683796 -0.348215
1 -2.407068 0.295611 -1.073675
8 -0.084099 2.242812 -2.130039
7 -0.722166 -1.025101 -3.574620
6 -0.879520 -1.061550 -4.917502
8 -0.419674 -0.194815 -5.662603
6 -1.641535 -2.234193 -5.455803
1 -2.045684 -2.892044 -4.674285
1 -2.465289 -1.864340 -6.084810
1 -0.975982 -2.818323 -6.110332
1 -2.299288 1.837339 0.778862
12 0.179644 2.330821 -0.121127
8 2.038476 3.151136 0.150257
1 2.169649 3.868925 0.787633
8 -0.663058 4.115655 0.451105
1 -0.232999 4.934535 0.161297
1 2.780414 2.543349 0.288369
1 -1.609744 4.255854 0.297528
8 -1.909877 1.402130 -3.126412
1 -2.220732 2.276502 -2.834699

2-IM3

6 -0.870808 -0.049275 -2.466990
6 0.147802 0.716149 -1.971955
1 -1.707860 -0.473016 -4.326355
1 -1.801748 -0.151630 -1.905717
8 1.279487 0.971277 -2.533262
7 -0.867359 -0.616673 -3.767400
6 0.065487 -1.372658 -4.338229
8 1.147560 -1.674951 -3.766741
6 -0.192924 -1.872547 -5.716235
1 -1.203079 -1.642087 -6.079285
1 0.547301 -1.429234 -6.400746
1 -0.032162 -2.961037 -5.730695
12 2.451826 -0.586172 -2.760108
8 2.566152 -1.490126 -0.939388
1 3.200710 -1.141014 -0.294671
8 4.245450 -0.053290 -3.511916
1 4.729657 -0.660309 -4.092690
1 4.338851 0.822109 -3.918717
1 1.720396 -1.528521 -0.464210
8 -0.046462 1.237225 -0.726612
1 0.753640 1.740342 -0.507199 **2-TS3'**

6 -0.473459 -0.529319 -2.220902
6 0.352246 0.583567 -1.812734
1 -1.618638 -0.558351 -3.982240
1 -1.435516 -0.566131 -1.699852
8 1.473869 0.820817 -2.306528
7 -0.673452 -0.725804 -3.642564
6 0.203200 -1.114815 -4.565310
8 1.417001 -1.325821 -4.325281

6	-0.299664	-1.295917	-5.955385
1	-1.380412	-1.132051	-6.054085
1	0.238990	-0.602801	-6.619480
1	-0.049241	-2.316072	-6.283890
12	2.554600	-0.921109	-2.739183
8	1.496542	-2.115037	-1.564887
1	1.645778	-2.114282	-0.610191
8	4.374765	-0.429758	-3.465057
1	4.430163	0.235932	-4.168263
1	5.082406	-0.203406	-2.841969
1	0.415732	-1.479375	-1.758220
8	-0.061439	1.240142	-0.742339
1	0.656331	1.824742	-0.433573

2-TS3

6	-1.140560	-0.523239	-2.442693
6	-0.354050	0.587592	-1.960672
1	-1.789583	-0.703116	-4.433958
1	-2.201513	-0.452252	-2.181879
8	0.859993	0.722937	-2.207596
7	-0.986976	-0.885484	-3.835290
6	0.069214	-1.432094	-4.437384
8	1.151528	-1.674236	-3.856796
6	-0.063333	-1.751693	-5.887869
1	0.678161	-1.161309	-6.447808
1	0.192597	-2.811891	-6.034803
1	-1.065060	-1.556308	-6.292485
12	1.925119	-1.100612	-2.052048
8	2.903808	-0.540916	-0.307053
1	3.541344	0.187091	-0.368689
8	3.752211	-0.954215	-2.974900
1	4.579688	-0.984781	-2.472410
1	3.921792	-1.449602	-3.789883
1	-0.480401	-1.436135	-1.671736
8	0.458445	-2.066189	-1.069782
1	2.329879	-0.307015	0.438027
1	0.340405	-2.987887	-1.333731
8	-0.950595	1.364646	-1.068786
1	-0.280409	1.941296	-0.655865

2-IM4

6	-0.858963	-0.188103	-2.482154
6	0.103549	0.892659	-2.063061
1	-1.454585	-0.189342	-4.514821
1	-1.888042	0.127768	-2.277986
8	1.320241	0.774864	-2.160389
7	-0.742416	-0.541504	-3.878403
6	0.195096	-1.355985	-4.370925
8	1.114000	-1.808693	-3.655951
6	0.112536	-1.720338	-5.808348
1	-0.772738	-1.311797	-6.311581
1	1.023080	-1.360401	-6.311161
1	0.112163	-2.817689	-5.887432
12	2.426304	-0.970596	-2.381143
8	2.685464	-1.644100	-0.653331
1	3.182374	-2.454233	-0.507931
8	3.923649	-0.172312	-3.502055
1	4.583900	-0.757964	-3.902866
1	3.688662	0.460702	-4.197843
1	-0.637712	-1.067249	-1.851043
8	-0.464699	1.956194	-1.567961
1	0.217348	2.597243	-1.281830

AcGly

6	-0.267741	-0.213586	-2.263171
6	-0.982992	1.080722	-2.546572
1	-1.361298	-1.970561	-2.731634
1	0.814013	-0.027042	-2.371118
8	-1.916608	1.216774	-3.301179
7	-0.694457	-1.296543	-3.095425
6	-0.376582	-1.321686	-4.411007
8	0.352987	-0.467953	-4.913711
6	-0.959286	-2.443152	-5.211268
1	-1.469361	-3.198999	-4.598857
1	-1.677959	-2.022424	-5.931902
1	-0.157532	-2.918791	-5.794910
1	-0.430304	-0.462750	-1.203476
8	-0.454066	2.077316	-1.839938
1	-0.949325	2.894226	-2.034587

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