SUPPORTING INFORMATION

Glycerol-enabled glycolysis of TDI-based polyurethane foams for selective recovery of aromatic diamines

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Table S1 Comparison of Physical, Chemical, and Biological Recycling Routes for Polyurethane

Recycling Type	Method	Advantages	Disadvantages
Physical	Mechanical Recycling	- Low cost, simple equipment - Suitable for mass production - Can be recycled multiple times	- Performance degrades with cycles - Difficult to process dyed or filled waste - Limited to specific polyurethane types
	Re-bonding	- Simple process, low energy consumption - Suitable for low-performance products (e.g., carpet pads, soundproofing materials)	- Low product performance - Requires adhesives - Limited applications
Chemical	Glycolysis	- Recovers high-purity polyols - Suitable for closed-loop recycling (for new PU synthesis) - Mature industrial application	- High temperature required (180~250°C) - May produce carcinogenic aromatic amines (requires concentration control) - Complex and costly purification
	Hydrolysis	- Recovery of polyols and aniline monomers	- High energy consumption (300~400°C) - Byproducts require strict handling (e.g., amines) - Industrialization challenges
	Acidolysis/ Ammonolysis	- No aromatic amine pollution in products - Suitable for producing polyols for flexible foams	- Low reaction efficiency - Requires precise control of reaction conditions - Limited application scope
Biological	Microbial Degradation	- Environmentally friendly (no chemicals) - Fully mineralized into CO22/H22O - Suitable for lab or small-scale treatment	- Slow degradation (weeks to months) - Low efficiency for crosslinked/crystalline materials - Requires specific microbes/enzymes
	Enzymatic Degradation	- High selectivity - Mild conditions (room temperature/pressure)	- High enzyme cost - Limited scalability - Sensitivity to material structure

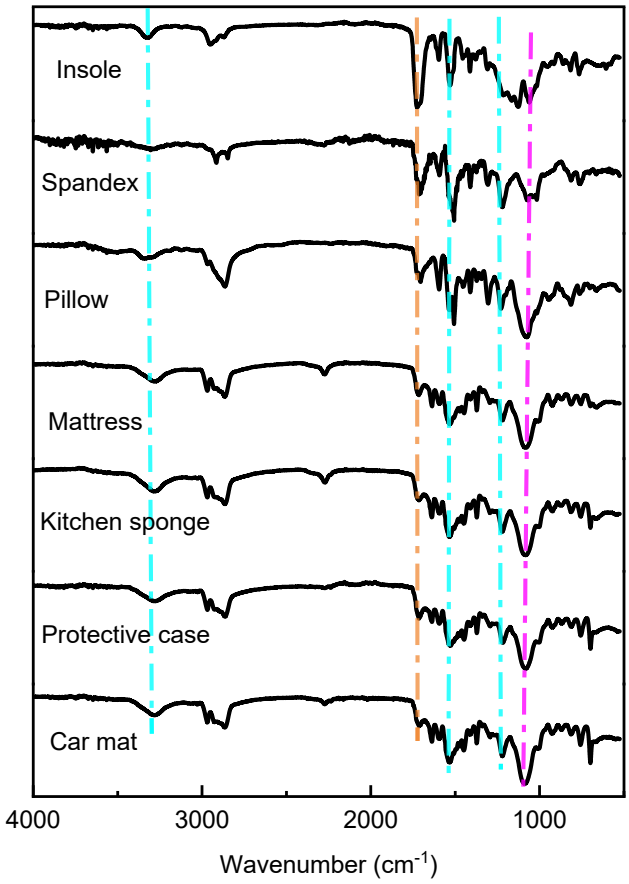
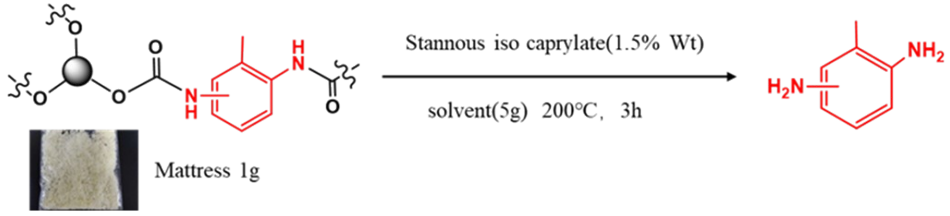
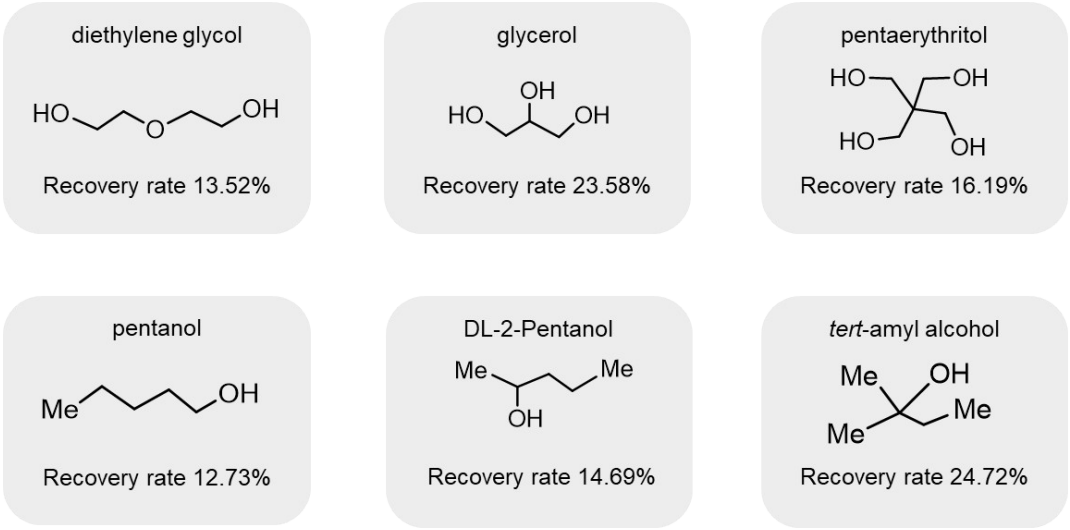


Figure S1. FTIR spectra of different commercial polyurethane (PU) samples.

All spectra display features typical of **aromatic PUs**: a broad **N–H stretch** at ~3300–3400 cm^{-1}, a **urethane C=O** band at ~1700–1730 cm^{-1}, and **aromatic ring** vibrations near ~1595 and ~1515 cm^{-1}. Samples dominated by **polyether soft segments** show pronounced **C–O–C** stretching around ~1100 cm^{-1} and relatively weaker ester carbonyl signals, whereas **polyester-rich** samples (e.g., *Kitchen sponge*) exhibit a stronger **ester C=O** near ~1728–1735 cm^{-1}. Molded elastomeric articles (e.g., *Insole, Spandex, Protective case*) tend to show **sharper carbonyl bands** (~1700–1715 cm^{-1}), more evident **urea/amide** contributions (amide I ~1640–1680 cm^{-1}; amide II ~1530–1550 cm^{-1}), and stronger **CH_2 bending** (~1410–1310 cm^{-1}), consistent with a higher hard-segment fraction.

Scheme S1. Aniline yields from alcoholysis of mattress polyurethane (PU) foam using different alcoholysis agents.





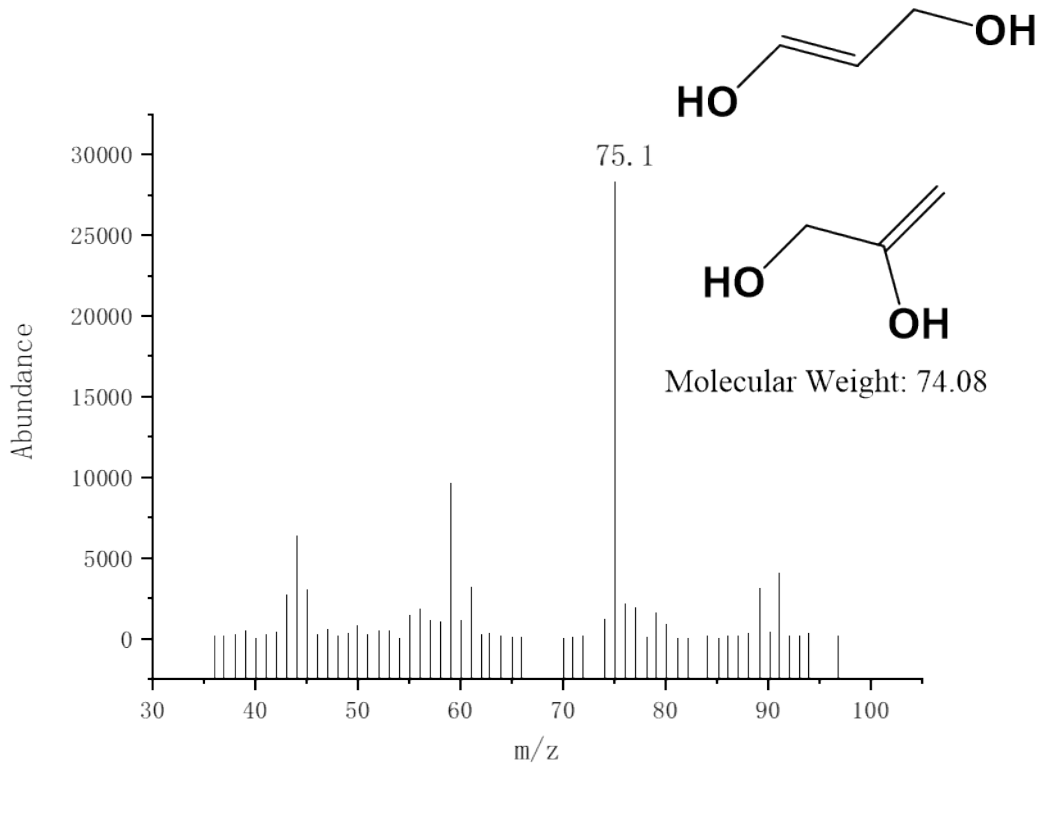


Figure S2. Detection of intermediate products from glycerolysis by LC-MS.

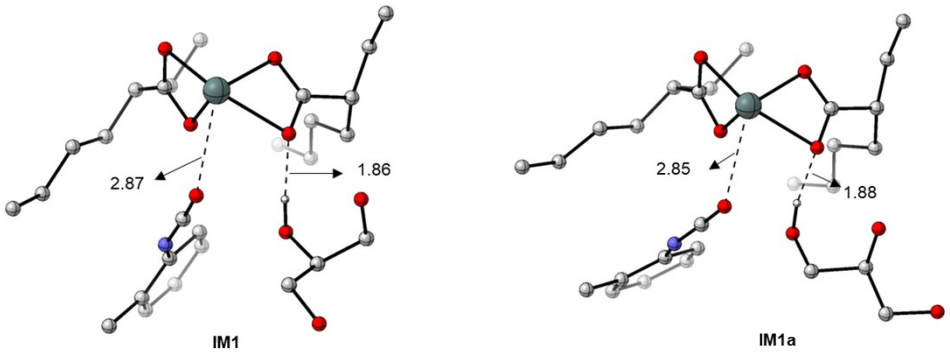


Figure S3. Optimized geometries along with the key bond distances in Å, part of the hydrogen atoms are omitted for clarity. (color code, C: grey, O: red, H: white, N: blue, Sn: dark gray).

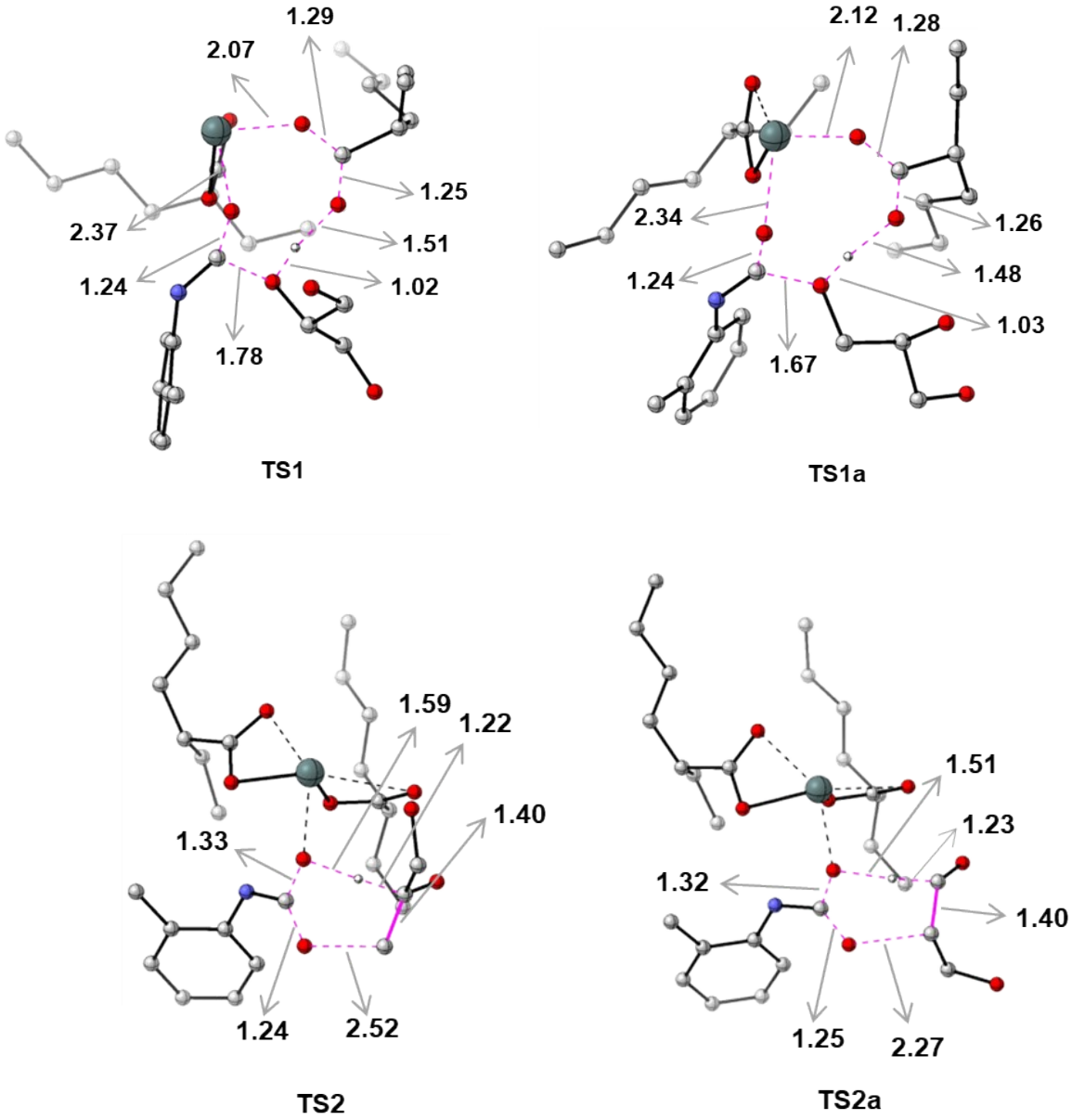


Figure S4. Optimized geometries along with the key bond distances in Å, part of the hydrogen atoms are omitted for clarity. (color code, C: grey, O: red, H: white, N: blue, Sn: dark gray).

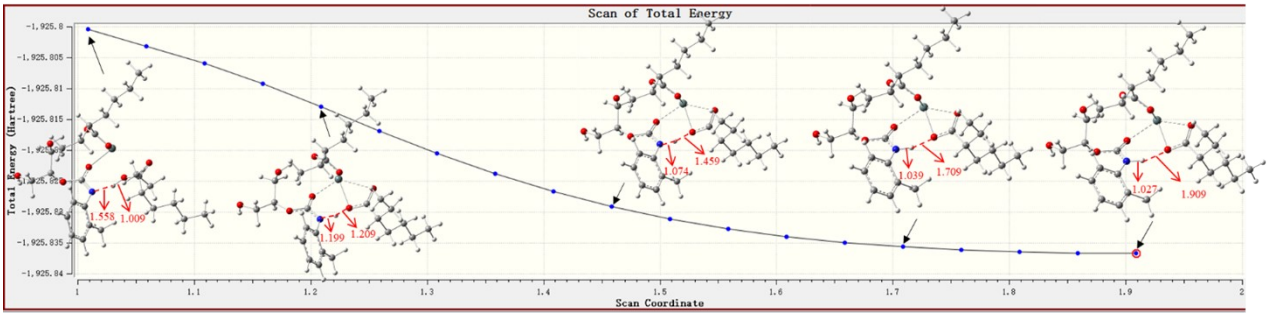


Figure S5. Scan of potential energy surface of the the H atom migrates from IM2 to IM3.

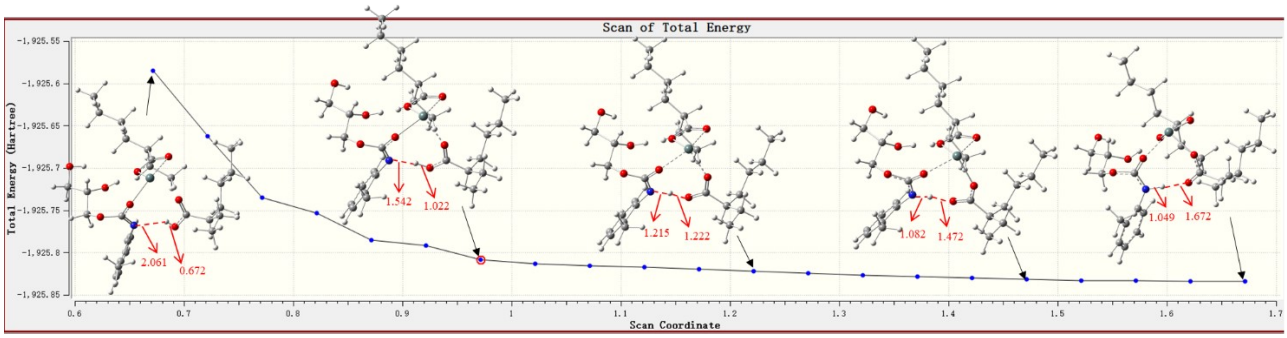


Figure S6. Scan of potential energy surface of the the H atom migrates from IM2a to IM3a.

Table S1 Coordinates and energies (in hatree) of the calculated structures at the B3LYP+(D3BJ)/6-311++G (d, p)//Lanl2DZ // B3LYP+(D3BJ)/6-31G (d,p)//Lanl2DZ level of theory.

Sn-Cat

Free Energy = -932.3507748 Hartree

Energy =-932.5953272 Hartree

Sn	-0.270749	-1.789722	-0.324830
O	1.120196	-1.668853	1.523722
O	-1.358976	-0.293529	0.816980
C	-1.626811	0.442299	-0.206757
C	1.795624	-0.779347	0.928499
O	1.424132	-0.435388	-0.259280
O	-1.219948	0.056363	-1.342040
C	2.974999	-0.108079	1.590611
H	3.092100	-0.614749	2.554091
C	-2.412126	1.721573	-0.046790
H	-2.488664	1.916158	1.028376
C	-1.671448	2.884780	-0.731951
H	-2.278780	3.788874	-0.608368
H	-1.620373	2.677564	-1.806845
C	-0.262927	3.121278	-0.182356
H	-0.288426	3.340538	0.890569
H	0.374505	2.243360	-0.332032
H	0.216071	3.967961	-0.685525
C	-3.829585	1.528611	-0.626648
H	-4.360833	2.483147	-0.527866
H	-3.742723	1.323363	-1.700896
C	-4.641404	0.419074	0.047978
H	-4.130116	-0.545601	-0.074811
H	-4.685739	0.606136	1.129742
C	-6.064290	0.301111	-0.507490
H	-6.014899	0.121095	-1.589958
H	-6.582226	1.261231	-0.379280
C	-6.874262	-0.811918	0.160564
H	-7.886577	-0.875473	-0.253709
H	-6.394680	-1.788052	0.020284
H	-6.965773	-0.640656	1.239810
C	2.638053	1.372594	1.867162
H	3.527296	1.838018	2.308875

H	2.448583	1.885522	0.919332
C	1.437828	1.551415	2.799841
H	0.521813	1.139372	2.363289
H	1.605358	1.047069	3.758677
H	1.259740	2.611843	3.006160
C	4.287036	-0.304833	0.794848
H	5.108123	-0.007234	1.459599
H	4.420190	-1.378348	0.606178
C	4.414419	0.459649	-0.527112
H	3.570987	0.210062	-1.179412
H	4.353569	1.539083	-0.339373
C	5.731323	0.154099	-1.249257
H	5.794827	-0.925349	-1.443884
H	6.574626	0.395772	-0.587659
C	5.877992	0.920242	-2.565732
H	6.823231	0.682590	-3.066446
H	5.063225	0.675172	-3.257607
H	5.853249	2.003582	-2.397332

1a

Free Energy = -439.1092993 Hartree

Energy = -439.2205147 Hartree

C	0.242435	-1.426151	-0.000522
C	1.589845	-1.778917	-0.000064
C	2.569242	-0.783940	0.000372
C	2.193794	0.560483	0.000282
C	0.848969	0.945305	-0.000175
C	-0.121535	-0.073720	-0.000496
H	-0.533187	-2.185881	-0.000907
H	1.869901	-2.827759	-0.000067
H	3.621160	-1.052333	0.000721
H	2.956285	1.334251	0.000551
C	0.438305	2.392827	-0.000074
H	-0.171503	2.632317	-0.878615
H	-0.167606	2.633230	0.880951
H	1.315207	3.044615	-0.002260
N	-1.467620	0.311995	-0.000903
C	-2.578021	-0.157657	0.000161
O	-3.714390	-0.478973	0.001130

2

Free Energy = -344.816409 Hartree

Energy = -344.9344901 Hartree

C	-1.199473	-0.766504	0.143575
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H	-1.216075	-0.915636	1.231762
C	0.027334	0.054843	-0.242482
H	0.090817	0.087126	-1.343472
C	1.301290	-0.575805	0.285517
H	1.287131	-1.651944	0.052031
H	1.318725	-0.467574	1.380182
O	-0.102363	1.371699	0.283439
H	-1.039496	1.589180	0.148014
O	2.419424	0.067255	-0.320024
H	3.216254	-0.320621	0.068652
O	-2.337564	-0.009691	-0.284278
H	-3.095936	-0.278472	0.252405

IM1

Free Energy =-1716.308052 Hartree

Energy = -1716.7817525 Hartree

Sn	1.239409	-1.018830	-2.239689
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O	0.442044	-3.098398	-1.561308
C	-0.288674	-2.510511	-0.715572
C	2.825684	-0.225814	-0.239715
O	2.750615	-1.426598	-0.654026
O	-0.191086	-1.223374	-0.627097
C	3.746191	0.201879	0.877427
H	4.223346	1.122186	0.514879
C	-1.233435	-3.264220	0.185077
H	-1.290508	-4.280629	-0.218821
C	-0.632822	-3.321688	1.607461
H	-1.341205	-3.867186	2.241561
H	-0.581625	-2.299825	1.997308
C	0.746799	-3.977270	1.682310
H	0.720715	-4.999659	1.288264
H	1.493131	-3.418507	1.108288
H	1.095032	-4.026212	2.719025
C	-2.632289	-2.624554	0.197626
H	-3.289085	-3.275896	0.787486
H	-2.575604	-1.669495	0.728478
C	-3.242181	-2.391353	-1.187213
H	-2.598134	-1.708290	-1.756404
H	-3.270461	-3.334700	-1.750089
C	-4.650108	-1.791513	-1.114801
H	-4.626557	-0.906927	-0.466605
H	-5.325961	-2.509229	-0.630643
C	-5.203884	-1.401652	-2.486261
H	-6.215828	-0.988750	-2.408971
H	-4.569428	-0.645020	-2.963280
H	-5.248156	-2.267246	-3.158318

C	4.832471	-0.837074	1.184999
H	5.329427	-0.533744	2.113934
H	4.364828	-1.807535	1.377906
C	5.870545	-0.973730	0.069120
H	5.406242	-1.299195	-0.867204
H	6.374448	-0.018347	-0.118416
H	6.636842	-1.709805	0.334697
C	2.898401	0.603361	2.112823
H	3.588291	1.035173	2.847453
H	2.205445	1.398174	1.820669
C	2.103672	-0.532092	2.763948
H	1.409238	-0.967664	2.033516
H	2.779242	-1.340357	3.069906
C	1.317742	-0.041160	3.985498
H	0.605615	0.731605	3.667535
H	2.012222	0.450223	4.680480
C	0.572543	-1.156897	4.720159
H	0.042496	-0.771183	5.598282
H	-0.166561	-1.638120	4.071410
H	1.265923	-1.933013	5.065668
C	0.756185	3.825266	0.168952
H	0.380651	4.448609	0.990428
C	2.275127	4.004003	0.115179
H	2.700866	3.669671	1.073537
O	2.895685	3.352461	-0.986485
H	2.707437	2.399709	-0.928343
O	0.374350	2.485109	0.486075
C	-1.992601	0.731537	1.642889
C	-2.438655	0.664403	2.960905
C	-3.737856	1.067312	3.279730
C	-4.586973	1.538440	2.276810
C	-4.167936	1.619061	0.943691
C	-2.855819	1.207259	0.647571
H	-0.993174	0.421144	1.368334
H	-1.772142	0.294368	3.732864
H	-4.089512	1.014091	4.305725
H	-5.597255	1.851534	2.525207
C	-5.074529	2.126559	-0.144791
H	-4.647837	3.008338	-0.636659
H	-5.221949	1.369407	-0.922825
H	-6.052491	2.398694	0.259698
N	-2.444089	1.261407	-0.686830
C	-1.493148	1.179679	-1.411188
O	-0.662082	1.126473	-2.259341
H	0.912359	1.865492	-0.036957
C	0.068034	4.270591	-1.120213
H	0.481949	3.701171	-1.962623
H	-1.004346	4.038064	-1.041894
H	2.491999	5.070534	0.005005
O	0.288383	5.670407	-1.274820
H	-0.005581	5.916312	-2.162462

IM1a

Free Energy = - 1716.3045902 Hartree

Energy = -1716.7797538 Hartree

Sn	0.810253	-1.697392	-1.997915
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O	-0.420672	-3.297220	-0.843247
C	-0.849509	-2.381618	-0.086099
C	2.746977	-1.091720	-0.241196
O	2.285629	-2.262137	-0.442586
O	-0.452332	-1.172419	-0.316355
C	3.847477	-0.817578	0.759296
H	4.673366	-0.403031	0.163453
C	-1.766802	-2.668498	1.076126
H	-2.018953	-3.732095	1.007381
C	-1.009795	-2.414939	2.396891
H	-1.707603	-2.607384	3.220011
H	-0.745686	-1.353866	2.445902
C	0.244591	-3.274125	2.564739
H	0.000236	-4.341804	2.520447
H	0.982483	-3.068999	1.782520
H	0.721296	-3.079583	3.530964
C	-3.056357	-1.833889	0.990506
H	-3.695519	-2.132214	1.830742
H	-2.810219	-0.777098	1.139105
C	-3.822718	-2.004021	-0.324596
H	-3.238396	-1.567604	-1.146632
H	-3.929897	-3.073454	-0.553933
C	-5.208001	-1.351137	-0.294452
H	-5.103272	-0.298864	-0.005354
H	-5.810871	-1.826234	0.491259
C	-5.942019	-1.446170	-1.633012
H	-6.922159	-0.958565	-1.588808
H	-5.366894	-0.966010	-2.433546
H	-6.101823	-2.491509	-1.923832
C	4.343407	-2.085200	1.471934
H	4.960302	-1.764213	2.319420
H	3.489852	-2.626630	1.892115
C	5.162324	-3.016682	0.575602
H	4.568409	-3.378241	-0.268424
H	6.042773	-2.500427	0.174968

H	5.514074	-3.888727	1.137571
C	3.391525	0.298402	1.729748
H	4.222920	0.499114	2.415205
H	3.229633	1.215055	1.157847
C	2.124523	-0.022126	2.527712
H	1.308601	-0.275760	1.838658
H	2.288450	-0.908808	3.152363
C	1.681859	1.152071	3.406172
H	1.505853	2.019389	2.758807
H	2.500683	1.424169	4.086237
C	0.419204	0.853054	4.216832
H	0.141871	1.701765	4.852349
H	-0.430312	0.637931	3.559567
H	0.560855	-0.017788	4.868402
C	1.241610	3.203056	-0.668064
H	0.723179	4.074736	-0.256673
H	0.933626	3.083747	-1.716569
C	2.753879	3.427567	-0.614687
H	3.051182	3.450084	0.447431
C	3.121790	4.768177	-1.230500
H	2.479455	5.548082	-0.793321
H	2.918629	4.729093	-2.311684
O	3.471352	2.415731	-1.313731
H	3.090269	1.544831	-1.107807
O	4.496546	5.032604	-0.969222
H	4.715906	5.865478	-1.409526
O	0.818048	2.091329	0.117678
C	-2.188694	1.962906	1.216988
C	-2.844144	2.296329	2.400823
C	-4.201431	2.625451	2.379702
C	-4.897995	2.631664	1.169496
C	-4.268765	2.305954	-0.037392
C	-2.905060	1.961581	0.013340
H	-1.131606	1.725616	1.195560
H	-2.291856	2.296634	3.335294
H	-4.716579	2.880284	3.301068
H	-5.952420	2.892732	1.153131
C	-5.008427	2.317996	-1.347610
H	-4.609816	3.088655	-2.018207
H	-4.908669	1.360922	-1.869200
H	-6.071551	2.517118	-1.192043
N	-2.284061	1.600074	-1.184010
C	-1.289542	1.218901	-1.726909
O	-0.393625	0.851382	-2.418917
H	1.197611	1.274527	-0.248663

TS1

Free Energy = -1716.2827942 Hartree

Energy = -1716.7543725 Hartree

Sn	-1.078942	0.463694	-2.073254
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O	-2.122109	1.684560	-0.333484
C	-0.993416	1.778198	0.224651
C	-1.988399	-1.807865	-0.132012
O	-2.095366	-1.135381	-1.232432
O	0.000358	1.157917	-0.320561
C	-3.171751	-2.683522	0.258619
H	-2.732140	-3.607860	0.653166
C	-0.755593	2.613462	1.459167
H	-1.732125	3.006432	1.761579
C	-0.173665	1.755580	2.599016
H	0.076840	2.430530	3.425654
H	0.765770	1.308787	2.255515
C	-1.123430	0.661476	3.089287
H	-2.073646	1.088119	3.430455
H	-1.337989	-0.064585	2.299954
H	-0.682847	0.111917	3.928414
C	0.177438	3.792473	1.108747
H	0.279397	4.409017	2.010011
H	1.174986	3.398190	0.881067
C	-0.308929	4.660808	-0.054753
H	-0.369378	4.055913	-0.970213
H	-1.329623	5.011828	0.150420
C	0.602357	5.863515	-0.318814
H	1.623018	5.505660	-0.510529
H	0.658163	6.479707	0.588711
C	0.131112	6.721903	-1.494409
H	0.799207	7.573957	-1.661897
H	0.097602	6.137184	-2.421495
H	-0.875982	7.117552	-1.316436
C	-4.092960	-3.037507	-0.914923
H	-4.980982	-3.535633	-0.506528
H	-4.438130	-2.119921	-1.400416
C	-3.426313	-3.949684	-1.947593
H	-2.546907	-3.470478	-2.389949
H	-3.101017	-4.891401	-1.489571
H	-4.116749	-4.195820	-2.761714
C	-3.907875	-1.999063	1.438777
H	-4.711595	-2.670674	1.765080
H	-3.205895	-1.916179	2.276616
C	-4.484590	-0.613905	1.129271
H	-3.689070	0.049716	0.769707

H	-5.215896	-0.685705	0.313880
C	-5.151779	0.030133	2.349000
H	-4.428671	0.067920	3.175001
H	-5.977618	-0.607082	2.693741
C	-5.672617	1.440284	2.063386
H	-6.143987	1.882527	2.948157
H	-4.857500	2.104181	1.751991
H	-6.416780	1.431905	1.257925
C	2.102180	-2.426013	0.836303
O	1.439054	-1.223161	0.366284
C	3.480760	1.064975	0.615516
C	4.402997	1.394153	1.607950
C	5.659392	0.783191	1.619857
C	5.985186	-0.155585	0.637612
C	5.079275	-0.500358	-0.372179
C	3.817212	0.123189	-0.363530
H	2.493660	1.512548	0.586892
H	4.137446	2.122556	2.368704
H	6.382313	1.033080	2.390847
H	6.959425	-0.637189	0.652045
C	5.401168	-1.530444	-1.421986
H	4.654376	-2.333055	-1.426657
H	5.392463	-1.089469	-2.426127
H	6.386045	-1.972176	-1.249790
N	2.909761	-0.180720	-1.395115
C	1.788663	-0.697035	-1.302315
O	0.791146	-0.990522	-1.970169
H	0.421839	-1.336673	0.418915
C	1.619888	-3.668122	0.093330
H	2.143184	-4.529834	0.515634
H	0.544863	-3.808002	0.268927
C	1.865803	-2.497699	2.342116
H	0.792717	-2.637318	2.537423
H	2.170622	-1.540214	2.787195
O	1.922773	-3.629414	-1.296283
H	1.287457	-3.033315	-1.719632
O	2.639424	-3.584206	2.836344
H	2.420097	-3.697619	3.771651
H	3.165384	-2.272421	0.642397

TS1a

Free Energy = -1716.2791493 Hartree

Energy = -1716.7514133 Hartree

Sn	1.087784	-2.109218	-1.794507
O	2.121993	1.154066	-1.618986
O	1.178979	-3.398135	0.185408
C	0.293375	-2.641224	0.671616
C	2.797241	0.352985	-0.913066
O	2.484203	-0.880929	-0.766703
O	-0.139589	-1.668399	-0.060201
C	4.010296	0.880039	-0.163312
H	4.601390	1.424420	-0.911694
C	-0.221453	-2.826893	2.079011
H	-0.078776	-3.887877	2.313286
C	0.658100	-1.990512	3.043343
H	0.235509	-2.109813	4.047816
H	0.547022	-0.932256	2.781103
C	2.139175	-2.369034	3.057159
H	2.275930	-3.423847	3.321740
H	2.605221	-2.209421	2.080802
H	2.681674	-1.766149	3.793061
C	-1.702945	-2.447377	2.234900
H	-2.006074	-2.725885	3.252194
H	-1.795518	-1.358601	2.170892
C	-2.658173	-3.083317	1.220732
H	-2.368323	-2.769935	0.211174
H	-2.565153	-4.178118	1.250154
C	-4.118738	-2.683372	1.460813
H	-4.177573	-1.591521	1.556057
H	-4.458095	-3.094452	2.421246
C	-5.053270	-3.141152	0.339421
H	-6.092179	-2.856736	0.540515
H	-4.763218	-2.689473	-0.617024
H	-5.023760	-4.230350	0.214399
C	4.885657	-0.219939	0.451313
H	5.621092	0.268409	1.101915
H	4.273091	-0.860650	1.092818
C	5.618782	-1.072692	-0.586721
H	4.915240	-1.600861	-1.237116
H	6.263801	-0.452334	-1.220365
H	6.251724	-1.823077	-0.100538
C	3.523699	1.926806	0.873816
H	4.404420	2.279162	1.423639
H	3.119756	2.793011	0.340900
C	2.468546	1.416589	1.861160
H	1.584854	1.069895	1.308237
H	2.849654	0.545147	2.406913
C	2.034353	2.493183	2.861398
H	1.696723	3.382945	2.313582
H	2.905787	2.808038	3.451303
C	0.922012	2.020306	3.799301
H	0.634743	2.805022	4.508120

H	0.025305	1.739131	3.234627
H	1.236023	1.145234	4.380172
C	-0.701664	2.749030	-1.345973
H	-1.711984	2.844749	-0.954304
H	-0.687305	2.983978	-2.413844
C	0.291541	3.617100	-0.572247
H	0.495356	3.107816	0.381067
C	-0.319369	4.969503	-0.238058
H	-1.308348	4.807186	0.214327
H	-0.458110	5.544631	-1.166377
O	1.489737	3.836801	-1.301057
H	1.923403	2.973370	-1.434180
O	0.558036	5.633040	0.663823
H	0.145768	6.475815	0.899715
O	-0.329871	1.347490	-1.153079
C	-2.581560	0.864599	0.697770
C	-3.313171	1.482398	1.710786
C	-4.583704	1.995336	1.439681
C	-5.114345	1.878801	0.152630
C	-4.401052	1.262594	-0.881404
C	-3.111932	0.763359	-0.598590
H	-1.600806	0.448674	0.891293
H	-2.892777	1.554440	2.709749
H	-5.160419	2.476823	2.223835
H	-6.105181	2.271882	-0.060029
C	-4.971155	1.139646	-2.268948
H	-4.366272	1.691035	-2.998695
H	-4.982955	0.094609	-2.599336
H	-5.992245	1.527946	-2.308496
N	-2.425045	0.094096	-1.621560
C	-1.206310	0.135178	-1.898766
O	-0.396725	-0.488693	-2.602830
H	0.649965	1.186641	-1.435969

IM2

Free Energy = -1716.3019784 Hartree

Energy = - 1716.7718095 Hartree

Sn	0.821237	-1.237535	-2.169809
O	2.401563	1.818177	-1.276615
O	1.372421	-3.215029	-0.638545
C	0.604236	-2.620261	0.144841
C	3.048191	0.740272	-0.928341
O	2.654745	-0.414619	-1.218092
O	0.151847	-1.436555	-0.174368
C	4.282376	0.974632	-0.093992
H	4.903678	1.677190	-0.664964
C	0.164137	-3.216821	1.466133
H	0.392981	-4.286617	1.402169
C	0.997748	-2.602599	2.613105
H	0.603028	-2.996801	3.557083
H	0.824975	-1.521015	2.628100
C	2.496046	-2.892050	2.519226
H	2.690819	-3.970708	2.531185
H	2.926525	-2.489938	1.597067
H	3.033433	-2.445253	3.362231
C	-1.342002	-3.020572	1.707124
H	-1.604385	-3.553728	2.629868
H	-1.533148	-1.958405	1.889125
C	-2.241768	-3.497001	0.562722
H	-1.995620	-2.933113	-0.345872
H	-2.037711	-4.553880	0.340152
C	-3.732919	-3.313234	0.865732
H	-3.908522	-2.276689	1.178000
H	-4.010689	-3.943489	1.721591
C	-4.630360	-3.638975	-0.329560
H	-5.689635	-3.501905	-0.084992
H	-4.399003	-2.987397	-1.180790
H	-4.495289	-4.676011	-0.660004
C	5.082233	-0.308024	0.164954
H	5.830235	-0.076342	0.931489
H	4.422467	-1.071030	0.588851
C	5.783760	-0.856513	-1.079630
H	5.065049	-1.125077	-1.859518
H	6.475738	-0.116411	-1.498270
H	6.362001	-1.754003	-0.835534
C	3.840259	1.707112	1.202734
H	4.730401	1.831508	1.829154
H	3.502844	2.713960	0.935513
C	2.737006	0.999899	1.999091
H	1.870256	0.806986	1.351871
H	3.088769	0.019093	2.339082
C	2.269074	1.830642	3.198610
H	1.940668	2.812938	2.836381
H	3.120978	2.015020	3.866819
C	1.135448	1.165843	3.981700
H	0.803989	1.794498	4.815700
H	0.266372	0.981747	3.339002
H	1.450503	0.201483	4.396458
C	-1.164157	3.233748	0.124333
H	-2.142328	2.940401	0.511088
C	-0.358546	3.914077	1.223080
H	-0.365517	3.274299	2.116431

O	0.971187	4.203768	0.805768
H	1.318552	3.388662	0.412490
O	-0.370224	2.068734	-0.208171
C	-2.573263	0.486196	1.171561
C	-3.564703	0.451365	2.150399
C	-4.909654	0.542553	1.784222
C	-5.245744	0.661868	0.433123
C	-4.267529	0.703259	-0.566640
C	-2.907690	0.626700	-0.187919
H	-1.528056	0.393781	1.443139
H	-3.284335	0.343572	3.194535
H	-5.689650	0.512668	2.539358
H	-6.291399	0.723669	0.141844
C	-4.639586	0.825850	-2.020500
H	-4.279551	1.768099	-2.450650
H	-4.185731	0.022015	-2.611399
H	-5.724382	0.785982	-2.152182
N	-1.939723	0.578371	-1.201293
C	-0.793847	1.140165	-1.116226
O	0.193929	0.835144	-1.941370
H	1.469352	1.552687	-1.631554
C	-1.335132	4.092254	-1.124000
H	-0.350353	4.458136	-1.442890
H	-1.754805	3.479518	-1.935009
H	-0.837094	4.863781	1.474646
O	-2.210933	5.154928	-0.768466
H	-2.188184	5.805552	-1.483690

IM2a

Free Energy = -1716.3001042 Hartree

Energy = -1716.771597 Hartree

Sn	0.439574	-1.942744	-1.939059
O	2.525797	0.878454	-1.781310
O	0.624097	-3.476736	-0.039802
C	-0.093232	-2.651718	0.575285
C	2.960504	-0.143403	-1.098674
O	2.333753	-1.229388	-1.032505
O	-0.418842	-1.543054	-0.023304
C	4.246752	0.076642	-0.345487
H	4.942914	0.523461	-1.066815
C	-0.562818	-2.894223	1.992173
H	-0.498224	-3.977182	2.146817
C	0.416280	-2.202621	2.970919
H	0.009613	-2.326573	3.981440
H	0.416280	-1.126831	2.762428
C	1.843641	-2.748137	2.918031
H	1.863423	-3.820198	3.145618
H	2.289861	-2.612589	1.928549
H	2.481942	-2.239454	3.647846
C	-2.007289	-2.424831	2.223984
H	-2.285004	-2.707343	3.247328
H	-2.037667	-1.331348	2.181741
C	-3.030443	-2.997346	1.238876
H	-2.774399	-2.673021	0.222300
H	-2.972992	-4.095041	1.241804
C	-4.465491	-2.560179	1.550971
H	-4.505508	-1.463893	1.586217
H	-4.742041	-2.911356	2.554464
C	-5.480642	-3.072664	0.527501
H	-6.498122	-2.749855	0.774796
H	-5.247691	-2.699422	-0.476996
H	-5.480284	-4.168423	0.481743
C	4.851393	-1.224205	0.197388
H	5.680719	-0.946167	0.857461
H	4.113511	-1.740946	0.818217
C	5.364563	-2.164321	-0.895638
H	4.556077	-2.490058	-1.557185
H	6.126926	-1.672611	-1.511106
H	5.816222	-3.060203	-0.456621
C	3.983595	1.144149	0.754306
H	4.913513	1.251909	1.324000
H	3.791384	2.109682	0.275138
C	2.822856	0.821747	1.701539
H	1.882115	0.798934	1.135178
H	2.949614	-0.177968	2.131479
C	2.695051	1.847940	2.832491
H	2.688991	2.858617	2.404449
H	3.586198	1.793001	3.471786
C	1.436980	1.646817	3.679193
H	1.363756	2.399161	4.472420
H	0.532446	1.722838	3.063626
H	1.431467	0.659619	4.154889
C	-0.463262	3.092463	-0.402447
H	-1.284882	3.117551	0.315338
H	-0.793823	3.523209	-1.353504
C	0.759029	3.817858	0.146718
H	1.008577	3.364134	1.116674
C	0.450601	5.284849	0.384083
H	-0.519468	5.365211	0.898109
H	0.360658	5.789101	-0.589742
O	1.860767	3.723775	-0.747135
H	1.986572	2.784886	-0.952349

O	1.498652	5.842518	1.168540
H	1.305279	6.783796	1.279868
O	-0.024570	1.734619	-0.623928
C	-2.741293	1.024614	0.662414
C	-3.726969	1.422121	1.565095
C	-4.880442	2.059848	1.101604
C	-5.033028	2.291827	-0.267986
C	-4.057281	1.902482	-1.192053
C	-2.889821	1.265577	-0.714783
H	-1.846986	0.515116	1.003469
H	-3.593604	1.229109	2.625998
H	-5.654897	2.370875	1.796593
H	-5.929746	2.786206	-0.633780
C	-4.222797	2.160759	-2.665940
H	-3.462946	2.858953	-3.038041
H	-4.102346	1.237187	-3.243735
H	-5.207621	2.583288	-2.883513
N	-1.952889	0.793488	-1.646055
C	-0.689889	0.922764	-1.494990
O	0.172753	0.227022	-2.221998
H	1.533164	0.696897	-2.064947

IM3

Free Energy = - 1716.3405801 Hartree

Energy = -1716.8089699 Hartree

Sn	-0.434758	-1.260211	-1.735659
O	1.043131	-2.868215	0.472228
C	0.385441	-1.957971	1.002638
O	-0.148203	-0.985738	0.314399
C	0.129044	-1.902438	2.502443
H	0.362189	-2.902518	2.885722
C	1.078115	-0.885983	3.175717
H	0.771449	-0.796200	4.224834
H	0.921016	0.098476	2.719983
C	2.557565	-1.265659	3.108721
H	2.731071	-2.248902	3.562006
H	2.929304	-1.309636	2.081124
H	3.168988	-0.537671	3.652904
C	-1.340877	-1.560826	2.805758
H	-1.480032	-1.617533	3.893050
H	-1.523737	-0.520774	2.516111
C	-2.366946	-2.458999	2.108918
H	-2.236511	-2.378598	1.023278
H	-2.185886	-3.509948	2.375228
C	-3.812340	-2.083794	2.452885
H	-3.967369	-1.020556	2.225155
H	-3.971069	-2.191824	3.534518
C	-4.845348	-2.919449	1.694191
H	-5.868716	-2.624805	1.952364
H	-4.727987	-2.799863	0.610578
H	-4.737833	-3.986819	1.921994
C	4.247905	-0.911688	-1.416520
H	4.175118	-0.696661	-2.488459
C	3.789707	-2.346062	-1.168324
O	3.452974	0.087590	-0.701432
C	2.947403	1.968823	1.443948
C	3.417785	2.925206	2.343024
C	3.099044	4.271292	2.159372
C	2.317861	4.655351	1.067978
C	1.845426	3.718947	0.141354
C	2.171195	2.364633	0.351528
H	3.177222	0.922219	1.587525
H	4.021778	2.612291	3.189337
H	3.457004	5.019913	2.859788
H	2.073808	5.703568	0.919247
C	1.022918	4.142536	-1.047804
H	0.951709	5.231502	-1.098349
H	1.462088	3.780519	-1.984394
H	0.002137	3.744369	-0.998873
N	1.633277	1.417367	-0.561591
C	2.217116	0.337385	-1.097665
O	1.626659	-0.383273	-1.946359
O	-0.944465	0.855374	-1.619684
C	-2.138120	0.740998	-1.108410
O	-2.624675	-0.406512	-0.985231
C	-2.851622	1.992595	-0.643862
H	-2.281719	2.837591	-1.044454
C	-2.791630	2.066381	0.900044
H	-3.393477	2.928177	1.212833
H	-3.271770	1.176019	1.318693
C	-1.371311	2.192474	1.454852
H	-0.760697	1.326349	1.185606
H	-0.875540	3.090635	1.072917
H	-1.387081	2.261116	2.547940
C	-4.293578	2.084981	-1.194810
H	-4.637114	3.113118	-1.021992
H	-4.260066	1.952415	-2.284291
C	-5.316322	1.110364	-0.599052
H	-4.948579	0.085853	-0.711835
H	-5.415705	1.290247	0.478854
C	-6.697373	1.234878	-1.250444
H	-6.607211	1.048770	-2.329527

H	-7.060313	2.266889	-1.147020
C	-7.720703	0.268908	-0.648658
H	-8.698959	0.363730	-1.133128
H	-7.392299	-0.771610	-0.759389
H	-7.859518	0.457942	0.422644
H	0.672393	1.553040	-0.882924
H	2.809379	-2.504617	-1.621090
O	3.780436	-2.683527	0.206346
H	2.846239	-2.819114	0.451584
C	5.670203	-0.646855	-0.916935
H	5.895261	0.423407	-1.016090
H	5.726680	-0.912762	0.142262
O	6.616455	-1.457997	-1.595884
H	6.663152	-1.148538	-2.512873
H	4.514314	-2.978019	-1.699700

IM3a

Free Energy = -1716.3388136 Hartree

Energy = -1716.809454 Hartree

Sn	-0.206023	-1.319208	-1.554839
O	1.270596	-2.640216	0.846778
C	0.608479	-1.669890	1.248124
O	0.098811	-0.779646	0.438542
C	0.300430	-1.445532	2.722857
H	0.622242	-2.356384	3.240402
C	1.098766	-0.248953	3.282683
H	0.726400	-0.048842	4.294831
H	0.867694	0.639358	2.684007
C	2.610618	-0.471769	3.329619
H	2.857517	-1.356558	3.928772
H	3.035596	-0.618787	2.332627
H	3.115231	0.387183	3.785231
C	-1.211334	-1.240361	2.937138
H	-1.391169	-1.191265	4.018804
H	-1.493175	-0.266395	2.523603
C	-2.100868	-2.320760	2.316141
H	-1.953696	-2.326805	1.229456
H	-1.799386	-3.311367	2.684871
C	-3.589330	-2.097519	2.603140
H	-3.866970	-1.086565	2.276601
H	-3.760081	-2.126552	3.687943
C	-4.493875	-3.119605	1.911759
H	-5.551525	-2.931154	2.127678
H	-4.365318	-3.085913	0.823392
H	-4.262987	-4.140320	2.239755
C	4.378859	-0.490865	-1.489324
H	5.388548	-0.208944	-1.185218
H	4.314461	-0.485063	-2.579740
C	4.009608	-1.866814	-0.932999
C	5.088670	-2.868952	-1.329561
H	6.003144	-2.644325	-0.760414
H	5.322164	-2.761293	-2.401006
O	4.595616	-4.171086	-1.035660
H	5.315283	-4.796957	-1.196544
O	3.569413	0.594825	-0.962190
C	2.883218	2.481150	1.145084
C	3.273921	3.533213	1.972156
C	2.821308	4.828011	1.713102
C	1.987561	5.064920	0.619011
C	1.592628	4.030294	-0.237345
C	2.052874	2.730752	0.048862
H	3.215585	1.470746	1.343949
H	3.920785	3.335451	2.821487
H	3.116312	5.650833	2.357405
H	1.639529	6.073144	0.411921
C	0.710429	4.296772	-1.429297
H	0.553254	5.370011	-1.559724
H	1.152906	3.896722	-2.348546
H	-0.274460	3.827291	-1.318610
N	1.594601	1.672568	-0.782640
C	2.280796	0.622599	-1.251774
O	1.734841	-0.266869	-1.958883
O	-0.931444	0.731278	-1.667400
C	-2.103744	0.565462	-1.121488
O	-2.475662	-0.598094	-0.848363
C	-2.932685	1.791807	-0.802709
H	-2.437356	2.634242	-1.296806
C	-2.895180	2.044160	0.722255
H	-3.575295	2.877001	0.938122
H	-3.295342	1.166015	1.239270
C	-1.495922	2.360681	1.255016
H	-0.803535	1.534227	1.071765
H	-1.086141	3.258467	0.781246
H	-1.523139	2.538166	2.335539
C	-4.370235	1.689632	-1.363740
H	-4.811399	2.692706	-1.298507
H	-4.310235	1.450554	-2.433778
C	-5.303537	0.687407	-0.674667
H	-4.839411	-0.303563	-0.682458
H	-5.432183	0.964466	0.379335
C	-6.682407	0.613142	-1.338280
H	-6.561982	0.330972	-2.393296

H	-7.144021	1.610314	-1.338747
C	-7.615015	-0.383388	-0.645739
H	-8.592096	-0.432253	-1.139315
H	-7.186820	-1.393066	-0.652122
H	-7.783890	-0.104210	0.401264
H	0.608683	1.661819	-1.052799
H	3.067845	-2.194756	-1.380610
O	3.877638	-1.792647	0.476079
H	3.054741	-2.259824	0.708023

TS2

Free Energy = -1716.273937 Hartree

Energy = -1716.7476835 Hartree

Sn	-0.171038	-1.120450	-1.790219
O	0.814118	-2.990549	0.270157
C	0.346386	-2.021117	0.905372
O	-0.102500	-0.964011	0.307811
C	0.245218	-2.005366	2.420332
H	0.518647	-3.010306	2.760256
C	1.242716	-0.983104	3.006334
H	1.131181	-0.997637	4.097134
H	0.947063	0.018004	2.672300
C	2.702551	-1.241944	2.630610
H	3.019472	-2.247175	2.931030
H	2.866364	-1.154037	1.553125
H	3.362610	-0.520869	3.124701
C	-1.195109	-1.674876	2.859839
H	-1.252569	-1.796477	3.948931
H	-1.384602	-0.616975	2.647810
C	-2.282623	-2.515600	2.184000
H	-2.224285	-2.370966	1.098064
H	-2.104570	-3.583494	2.372972
C	-3.694588	-2.138771	2.645228
H	-3.842285	-1.061342	2.490358
H	-3.785096	-2.308523	3.726759
C	-4.790276	-2.911094	1.907574
H	-5.789338	-2.610173	2.242223
H	-4.734367	-2.735042	0.826800
H	-4.694299	-3.991180	2.071497
C	4.675198	-1.513689	-1.412531
H	4.884248	-1.048380	-2.373050
C	3.612944	-2.419424	-1.366271
O	3.606038	0.601419	-0.564389
C	2.843460	2.670529	1.358059
C	3.157635	3.767668	2.159298
C	2.594596	5.016274	1.890389
C	1.727188	5.159296	0.805758
C	1.408972	4.079641	-0.025952
C	1.973720	2.820732	0.270054
H	3.271143	1.697522	1.561364
H	3.834037	3.639786	2.999597
H	2.830469	5.872735	2.515122
H	1.293032	6.130910	0.584778
C	0.501191	4.257270	-1.215614
H	0.250801	5.311752	-1.355689
H	0.974322	3.889220	-2.133569
H	-0.437114	3.703156	-1.101107
N	1.602646	1.720479	-0.533661
C	2.409026	0.677447	-0.886457
O	1.837769	-0.254954	-1.638602
O	-0.917940	0.909134	-1.584020
C	-2.122051	0.664973	-1.139757
O	-2.527013	-0.516490	-1.106979
C	-2.947484	1.829239	-0.629901
H	-2.469272	2.738892	-1.007401
C	-2.873599	1.859507	0.915827
H	-3.554948	2.646059	1.262511
H	-3.258648	0.912512	1.307721
C	-1.468412	2.106896	1.467953
H	-0.780218	1.309686	1.175518
H	-1.062078	3.057320	1.107549
H	-1.486789	2.147982	2.562590
C	-4.400444	1.800920	-1.156807
H	-4.834429	2.789283	-0.956477
H	-4.374048	1.694258	-2.249317
C	-5.321024	0.725209	-0.567670
H	-4.863837	-0.258196	-0.712628
H	-5.415783	0.870946	0.515737
C	-6.720490	0.739471	-1.190670
H	-6.636615	0.586320	-2.275460
H	-7.172160	1.732122	-1.055716
C	-7.640879	-0.327630	-0.593330
H	-8.635154	-0.307316	-1.053498
H	-7.225807	-1.332152	-0.739300
H	-7.769723	-0.178575	0.485545
H	0.647653	1.687881	-0.886805
H	2.883736	-1.448141	-1.479158
O	3.426793	-3.143768	-0.212556
H	2.461999	-3.209322	-0.021997
C	5.616776	-1.255223	-0.281852
H	5.945702	-0.215699	-0.254752
H	5.174130	-1.534761	0.672666

O	6.688318	-2.171207	-0.550722
H	7.260039	-1.766018	-1.222006
H	3.356516	-2.914441	-2.314636

TS2a

Free Energy = -1716.2702361 Hartree

Energy = -1716.7430705 Hartree

Sn	0.039908	-1.365024	-1.448882
O	0.737231	-2.932013	1.069507
C	0.376220	-1.794234	1.421026
O	0.170686	-0.827945	0.574394
C	0.119529	-1.434917	2.876588
H	0.289637	-2.350310	3.454253
C	1.107898	-0.347070	3.342328
H	0.841008	-0.064079	4.367938
H	0.958896	0.542640	2.720543
C	2.574419	-0.778666	3.290814
H	2.754805	-1.640790	3.944109
H	2.879562	-1.070076	2.280743
H	3.232001	0.032619	3.621786
C	-1.339365	-0.972189	3.061967
H	-1.518021	-0.841745	4.136998
H	-1.451745	0.014063	2.599388
C	-2.387998	-1.919383	2.471563
H	-2.232001	-1.994628	1.388405
H	-2.255317	-2.929366	2.884268
C	-3.823856	-1.446828	2.722058
H	-3.932594	-0.422436	2.341721
H	-4.008533	-1.393184	3.803647
C	-4.872424	-2.345898	2.063878
H	-5.888085	-1.972169	2.235628
H	-4.717082	-2.401629	0.980060
H	-4.821644	-3.368491	2.456923
C	4.835224	-1.494815	-0.663054
H	5.229043	-1.091397	0.260580
H	5.323484	-1.223383	-1.590741
C	3.813948	-2.445752	-0.660632
C	3.725400	-3.461395	-1.796652
H	4.343078	-4.329647	-1.531788
H	4.118827	-3.015673	-2.719499
O	2.355239	-3.817931	-1.916008
H	2.292850	-4.610205	-2.467585
O	3.885764	0.564323	-0.668129
C	3.041891	2.756834	1.140939
C	3.373164	3.930337	1.816696
C	2.896086	5.159080	1.356019
C	2.099607	5.204468	0.210429
C	1.768107	4.042762	-0.497304
C	2.244468	2.809797	-0.008458
H	3.397344	1.796530	1.493965
H	3.992555	3.880267	2.707481
H	3.143794	6.076427	1.881967
H	1.733750	6.159741	-0.156624
C	0.935114	4.104468	-1.751175
H	0.765503	5.141222	-2.052122
H	1.425250	3.578141	-2.578223
H	-0.044092	3.632074	-1.612592
N	1.856689	1.625442	-0.678841
C	2.664393	0.563017	-0.931350
O	2.094078	-0.484815	-1.507582
O	-0.631531	0.698910	-1.632832
C	-1.849037	0.591926	-1.172169
O	-2.296921	-0.541099	-0.896626
C	-2.641004	1.865525	-0.949707
H	-2.097622	2.661943	-1.468531
C	-2.645681	2.199549	0.560209
H	-3.293040	3.073071	0.705083
H	-3.106366	1.370562	1.106751
C	-1.254864	2.479938	1.132980
H	-0.598743	1.611423	1.028149
H	-0.780463	3.325658	0.625444
H	-1.316802	2.724206	2.199032
C	-4.062493	1.792854	-1.552851
H	-4.461002	2.815915	-1.557820
H	-3.980057	1.491966	-2.605716
C	-5.063025	0.872834	-0.843449
H	-4.650706	-0.139527	-0.795919
H	-5.200683	1.203937	0.193643
C	-6.428995	0.842227	-1.536547
H	-6.301551	0.508800	-2.575719
H	-6.835444	1.861774	-1.590082
C	-7.430105	-0.071751	-0.826006
H	-8.400672	-0.080170	-1.334643
H	-7.063694	-1.104641	-0.789742
H	-7.597997	0.254489	0.207531
H	0.892965	1.544450	-1.004784
H	3.066109	-1.562687	-1.082904
O	3.407976	-2.904486	0.582067
H	2.441368	-3.078494	0.577810

IM4

Free Energy = -1792.784296 Hartree

Energy = -1793.2865415 Hartree

Sn	-0.583298	-0.959922	-1.864172
O	2.331238	-0.586698	-0.026349
C	1.447471	-1.299555	0.500265
O	0.318871	-1.576314	-0.063896
C	1.707233	-1.978075	1.835595
H	2.455321	-1.363972	2.350150
C	0.452052	-2.113979	2.709909
H	0.740666	-2.646126	3.624587
H	-0.270471	-2.749670	2.187335
C	-0.206430	-0.783931	3.075176
H	0.503875	-0.106088	3.560249
H	-0.595233	-0.284944	2.184918
H	-1.044532	-0.936963	3.762985
C	2.323798	-3.372688	1.557967
H	2.532318	-3.832496	2.532128
H	1.561607	-3.997396	1.074315
C	3.600575	-3.380440	0.712048
H	3.384089	-3.009612	-0.297018
H	4.332470	-2.684103	1.143575
C	4.225749	-4.775221	0.604025
H	3.483448	-5.472403	0.191838
H	4.467111	-5.143957	1.610200
C	5.484455	-4.795945	-0.265880
H	5.913731	-5.802149	-0.327945
H	5.263363	-4.464189	-1.287477
H	6.255213	-4.128774	0.138389
C	2.590485	2.751520	-1.905435
H	1.985869	2.771427	-2.818341
C	3.567545	1.578015	-1.955042
O	1.708418	2.646811	-0.755377
C	1.731323	2.349323	2.092273
C	2.053916	2.914397	3.324133
C	1.050949	3.471958	4.120432
C	-0.269724	3.469883	3.670958
C	-0.619862	2.922555	2.430305
C	0.404378	2.359493	1.648234
H	2.500528	1.907885	1.471280
H	3.085435	2.907442	3.663031
H	1.295342	3.907952	5.084487
H	-1.051839	3.906914	4.285704
C	-2.047987	2.926685	1.951965
H	-2.671108	3.547301	2.600266
H	-2.125997	3.307281	0.927690
H	-2.472820	1.916442	1.951187
N	0.042134	1.730603	0.424971
C	0.720538	1.768956	-0.730747
O	0.419397	1.063607	-1.728984
O	-1.926954	0.018222	-0.425627
C	-2.695897	-0.968118	-0.040909
O	-2.539800	-2.102490	-0.525187
C	-3.781606	-0.630761	0.969549
H	-3.268926	-0.134511	1.804084
C	-4.490737	-1.880849	1.507192
H	-5.381251	-1.556137	2.059506
H	-4.841008	-2.487876	0.666422
C	-3.606088	-2.733681	2.419417
H	-2.719101	-3.083450	1.883702
H	-3.272888	-2.161494	3.293112
H	-4.147534	-3.613385	2.784964
C	-4.746536	0.408221	0.350509
H	-5.470129	0.700303	1.121615
H	-4.171758	1.305582	0.097382
C	-5.493976	-0.078207	-0.895297
H	-4.770917	-0.402867	-1.656680
H	-6.096858	-0.961430	-0.649030
C	-6.402153	0.998673	-1.497603
H	-5.797393	1.880913	-1.748082
H	-7.124443	1.327915	-0.738160
C	-7.150827	0.519941	-2.743190
H	-7.791178	1.308038	-3.154805
H	-6.451752	0.213215	-3.530460
H	-7.788734	-0.342025	-2.513814
H	-0.816377	1.170156	0.383858
H	3.046412	0.693348	-2.327070
O	4.191119	1.331372	-0.708206
H	3.644667	0.667706	-0.252002
C	3.291606	4.095337	-1.695387
H	2.538011	4.877479	-1.532868
H	3.916483	4.030425	-0.799975
O	4.156069	4.400789	-2.779034
H	3.602510	4.582591	-3.553287
H	4.337680	1.844031	-2.687582
O	1.925363	-1.639489	-2.473386
H	2.322261	-1.196976	-1.691122
H	2.332551	-1.236991	-3.253832

TS2-1

Free Energy = -1792.7171614 Hartree

Energy = -1793.22446 Hartree

Sn	-0.571528	-1.202841	-1.617304
O	2.502137	-1.364824	-0.693513

C	1.747382	-1.330546	0.307559
O	0.462399	-1.265085	0.226463
C	2.328382	-1.443374	1.708983
H	3.354626	-1.061233	1.653545
C	1.538630	-0.637085	2.750053
H	2.017203	-0.793850	3.724286
H	0.526733	-1.049845	2.822688
C	1.461475	0.858258	2.444133
H	2.461139	1.300219	2.361406
H	0.931204	1.037412	1.506019
H	0.925048	1.395829	3.233360
C	2.384667	-2.940806	2.098025
H	2.740324	-2.993690	3.134590
H	1.361497	-3.339015	2.098140
C	3.279723	-3.812707	1.213384
H	2.920140	-3.789967	0.177626
H	4.293279	-3.388305	1.192910
C	3.346135	-5.266658	1.692129
H	2.330076	-5.683401	1.720724
H	3.716794	-5.291858	2.725908
C	4.234178	-6.144428	0.807639
H	4.264506	-7.178350	1.169096
H	3.866938	-6.162977	-0.225478
H	5.264196	-5.768734	0.785280
C	4.301920	2.179762	-1.456805
H	4.268933	2.882348	-2.287547
C	4.629949	0.845833	-1.761259
O	1.717144	2.348398	-1.316057
C	0.646561	3.912219	0.928369
C	0.537492	5.045672	1.733272
C	-0.705542	5.645446	1.936804
C	-1.834682	5.099786	1.322553
C	-1.752823	3.970608	0.500928
C	-0.487068	3.370731	0.308006
H	1.600789	3.431435	0.782053
H	1.427645	5.450073	2.206964
H	-0.798042	6.526629	2.564741
H	-2.806788	5.562991	1.470755
C	-2.983765	3.417501	-0.171071
H	-3.840931	4.075481	-0.008386
H	-2.835079	3.307778	-1.251929
H	-3.249448	2.426443	0.213394
N	-0.425227	2.211927	-0.489834
C	0.624904	1.767904	-1.259411
O	0.344161	0.694728	-1.982534
O	-2.042913	-0.090316	-0.560089
C	-2.635194	-0.953293	0.232202
O	-2.356014	-2.159079	0.158480
C	-3.673428	-0.384680	1.183490
H	-3.274408	0.577077	1.528339
C	-3.890832	-1.291571	2.401076
H	-4.743275	-0.900665	2.970212
H	-4.165049	-2.295058	2.061440
C	-2.658843	-1.377305	3.305560
H	-1.809221	-1.804721	2.764190
H	-2.363797	-0.385137	3.667757
H	-2.851403	-2.008768	4.179750
C	-4.971127	-0.081265	0.393824
H	-5.667222	0.422287	1.076124
H	-4.732780	0.637612	-0.398970
C	-5.656028	-1.303958	-0.225274
H	-4.946319	-1.839440	-0.869859
H	-5.944781	-2.009604	0.563893
C	-6.896468	-0.930939	-1.043651
H	-6.606966	-0.228263	-1.836925
H	-7.605483	-0.391780	-0.400616
C	-7.589225	-2.146294	-1.663533
H	-8.470431	-1.853233	-2.245058
H	-6.911458	-2.687126	-2.334878
H	-7.919204	-2.850203	-0.890136
H	-1.257618	1.629467	-0.528532
H	3.678465	0.568861	-2.419281
O	4.837988	-0.047056	-0.719900
H	4.045606	-0.630382	-0.638086
C	4.189078	2.721774	-0.077745
H	3.511523	3.569967	-0.004901
H	3.937551	1.951902	0.648846
O	5.566542	3.093598	0.117461
H	5.689182	3.979217	-0.262461
H	5.371805	0.773728	-2.574740
O	2.530418	-0.276611	-3.200552
H	2.506360	-0.950352	-2.490950
H	1.753507	0.274198	-2.934766

IM5

Free Energy = -1792.7724081 Hartree

Energy = -1793.2814266 Hartree

Sn	-0.795490	-0.991833	-1.642386
O	2.121375	-2.045304	-0.485320
C	1.328036	-1.694814	0.416985
O	0.189019	-1.122292	0.188872
C	1.641261	-1.922975	1.885791

H	2.554997	-2.526411	1.926680
C	1.897780	-0.571486	2.586275
H	1.996949	-0.770687	3.659792
H	1.008510	0.057463	2.461152
C	3.139460	0.164237	2.081366
H	4.038023	-0.449401	2.201020
H	3.059250	0.422616	1.021710
H	3.286939	1.095281	2.637954
C	0.492024	-2.690433	2.564707
H	0.791221	-2.890341	3.600924
H	-0.386616	-2.037154	2.606726
C	0.116040	-4.004903	1.875679
H	-0.211797	-3.800093	0.847281
H	1.003891	-4.647569	1.795849
C	-0.999096	-4.761197	2.604701
H	-1.875262	-4.105529	2.697339
H	-0.673782	-4.985646	3.629519
C	-1.402256	-6.056570	1.897518
H	-2.200579	-6.577357	2.437824
H	-1.763650	-5.854898	0.881952
H	-0.551722	-6.743880	1.815364
C	5.909323	-0.572026	-1.982658
H	6.231154	-0.653675	-3.018881
C	5.178031	-1.579724	-1.479321
O	2.541852	1.969462	-0.978643
C	1.834672	3.563009	1.352673
C	1.983730	4.548041	2.329013
C	0.897803	5.338447	2.704162
C	-0.336588	5.141161	2.082875
C	-0.516370	4.168496	1.094050
C	0.590166	3.365102	0.739169
H	2.674880	2.952958	1.055593
H	2.954037	4.689004	2.796438
H	1.008665	6.104413	3.465867
H	-1.186038	5.760433	2.358686
C	-1.853946	3.998976	0.420334
H	-2.547457	4.779133	0.742473
H	-1.764839	4.050581	-0.671349
H	-2.310216	3.032350	0.657427
N	0.384492	2.361710	-0.235421
C	1.337082	1.771772	-1.000997
O	0.782865	0.885461	-1.890026
O	-1.875702	0.628645	-0.690157
C	-2.705226	-0.143889	-0.059479
O	-2.598472	-1.385760	-0.256290
C	-3.762218	0.467231	0.826332
H	-3.234494	1.194374	1.456354
C	-4.438050	-0.569726	1.733771
H	-5.292904	-0.081989	2.216835
H	-4.839720	-1.384112	1.122999
C	-3.498647	-1.139113	2.799348
H	-2.652472	-1.656202	2.338248
H	-3.100131	-0.344137	3.440749
H	-4.020820	-1.856737	3.441323
C	-4.753505	1.266582	-0.057478
H	-5.463797	1.762773	0.614265
H	-4.198634	2.057908	-0.573430
C	-5.517202	0.429070	-1.087958
H	-4.806923	-0.084452	-1.751095
H	-6.089203	-0.358434	-0.581783
C	-6.469186	1.274604	-1.940248
H	-5.895951	2.063657	-2.445557
H	-7.183165	1.787465	-1.281680
C	-7.230914	0.448591	-2.978698
H	-7.903231	1.075434	-3.574894
H	-6.540799	-0.050764	-3.669263
H	-7.837516	-0.328223	-2.498090
H	-0.565979	2.029501	-0.377892
H	3.462986	-0.350516	-2.694121
O	4.784401	-1.638681	-0.182409
H	3.876635	-2.013403	-0.146430
C	6.349286	0.630106	-1.198552
H	6.090138	1.547789	-1.749615
H	5.825582	0.660552	-0.240410
O	7.749405	0.623326	-0.879455
H	8.229283	0.600196	-1.720212
H	4.880490	-2.420809	-2.108486
O	2.549986	-0.666765	-2.814022
H	2.416153	-1.287983	-2.060574
H	1.564202	0.400044	-2.353883

IM4a

Free Energy = -1792.7877175 Hartree

Energy = -1793.2902461 Hartree

Sn	0.596236	0.882287	-1.783901
O	-2.286318	2.068893	0.043154
C	-1.174356	1.996842	0.619264
O	-0.074692	1.635178	0.054114
C	-1.035753	2.374055	2.087476
H	-2.028281	2.694041	2.423983
C	-0.590762	1.149384	2.907216
H	-0.422178	1.470770	3.941901

H	0.373186	0.805204	2.517189
C	-1.602922	0.004712	2.871724
H	-2.570758	0.315845	3.282053
H	-1.773538	-0.340817	1.848539
H	-1.251627	-0.853510	3.453151
C	-0.045684	3.544747	2.230009
H	0.030227	3.798765	3.294666
H	0.944890	3.200982	1.910645
C	-0.435723	4.791852	1.431085
H	-0.504441	4.540852	0.363353
H	-1.439360	5.122053	1.733617
C	0.555161	5.947029	1.604765
H	1.556701	5.608632	1.306216
H	0.624024	6.207011	2.669825
C	0.172370	7.188948	0.797123
H	0.897281	7.998499	0.937439
H	0.127453	6.963824	-0.275207
H	-0.812256	7.567466	1.096827
C	-3.628929	-1.530303	-2.063226
H	-3.312496	-1.472156	-3.107745
C	-3.988599	-0.137892	-1.536684
O	-2.611899	-2.190972	-1.276711
C	-2.469036	-3.075091	1.435908
C	-2.846736	-4.056141	2.349985
C	-1.936642	-5.046125	2.727660
C	-0.652940	-5.049298	2.182222
C	-0.249518	-4.081905	1.252564
C	-1.180961	-3.093309	0.887609
H	-3.158763	-2.291430	1.145386
H	-3.847186	-4.038942	2.771895
H	-2.224284	-5.811618	3.442244
H	0.056279	-5.820089	2.471226
C	1.137925	-4.098822	0.666603
H	1.652937	-5.029082	0.918361
H	1.113408	-3.999719	-0.423987
H	1.743002	-3.269854	1.048995
N	-0.760881	-2.073168	-0.014239
C	-1.474799	-1.562536	-1.026466
O	-1.092758	-0.588949	-1.728339
O	1.493397	-0.598003	-0.422787
C	2.538039	0.026010	0.056232
O	2.796717	1.186196	-0.305653
C	3.424550	-0.763261	1.007753
H	2.748133	-1.325087	1.664178
C	4.305292	0.148260	1.871545
H	5.033966	-0.479312	2.399717
H	4.873367	0.820816	1.221599
C	3.505663	0.971923	2.883319
H	2.795990	1.631453	2.374983
H	2.938006	0.323924	3.561713
H	4.165051	1.597855	3.494809
C	4.232223	-1.802259	0.190368
H	4.782560	-2.434137	0.898777
H	3.524604	-2.456204	-0.331381
C	5.209289	-1.207153	-0.828861
H	4.670507	-0.534107	-1.509031
H	5.955688	-0.588416	-0.314845
C	5.928196	-2.282271	-1.650372
H	5.181232	-2.900236	-2.167174
H	6.466585	-2.957070	-0.970859
C	6.905513	-1.698029	-2.672493
H	7.404548	-2.486091	-3.247420
H	6.387978	-1.043181	-3.383771
H	7.682855	-1.101682	-2.179921
H	0.183265	-1.676758	0.075309
H	-3.291171	0.591894	-1.946077
O	-3.911660	-0.137782	-0.111618
H	-3.451923	0.686021	0.143317
O	-1.430266	2.339252	-2.437612
H	-1.948306	2.288579	-1.594083
H	-1.994093	1.976248	-3.135720
H	-4.483940	-2.201394	-1.976320
C	-5.416138	0.229404	-1.948684
H	-5.569003	0.061797	-3.020789
H	-5.571425	1.300852	-1.748625
O	-6.357308	-0.570308	-1.247239
H	-6.054349	-0.545306	-0.324582

TS2a-1

Free Energy = -1792.7150021 Hartree

Energy = -1793.2215772 Hartree

Sn	-0.590651	-0.891776	-1.686007
O	2.378410	-1.727159	-0.537874
C	1.527281	-1.612751	0.375680
O	0.300477	-1.269304	0.180811
C	1.884765	-1.920322	1.821895
H	2.963509	-2.109058	1.850713
C	1.551848	-0.729446	2.738057
H	1.800322	-1.017295	3.766442
H	0.470275	-0.556816	2.706070
C	2.291916	0.555249	2.364126
H	3.375581	0.401888	2.352744

H	1.999264	0.903041	1.369663
H	2.064635	1.359792	3.070731
C	1.140373	-3.195338	2.268105
H	1.426362	-3.403949	3.306500
H	0.063860	-2.985892	2.270809
C	1.419550	-4.427583	1.403075
H	1.108094	-4.233529	0.367466
H	2.502057	-4.613267	1.367720
C	0.701842	-5.683082	1.908467
H	-0.378287	-5.487232	1.949276
H	1.015858	-5.887705	2.940998
C	0.966789	-6.913317	1.038178
H	0.442614	-7.796131	1.420775
H	0.631498	-6.747161	0.007400
H	2.037010	-7.149899	1.003572
C	4.303496	1.875604	-0.602829
H	4.490714	2.724895	-1.248177
C	4.677070	0.586473	-1.006097
O	2.159412	2.418728	-1.172203
C	1.399612	3.921963	1.200555
C	1.433164	5.027996	2.048847
C	0.253321	5.689935	2.388578
C	-0.957285	5.236877	1.862106
C	-1.020143	4.136895	1.000069
C	0.182029	3.468042	0.674473
H	2.312468	3.410852	0.937636
H	2.386631	5.364074	2.446211
H	0.272810	6.550043	3.051241
H	-1.881634	5.751359	2.111551
C	-2.340236	3.691908	0.425348
H	-3.130755	4.399845	0.685458
H	-2.297271	3.612270	-0.667139
H	-2.638220	2.708720	0.803217
N	0.098174	2.334180	-0.162933
C	1.040891	1.876005	-1.045049
O	0.667656	0.865031	-1.796616
O	-1.912887	0.345473	-0.550715
C	-2.684581	-0.531383	0.044040
O	-2.552466	-1.739387	-0.220193
C	-3.729395	0.006839	1.002982
H	-3.228701	0.785776	1.591108
C	-4.243005	-1.074469	1.962504
H	-5.095037	-0.659975	2.515091
H	-4.619123	-1.924264	1.384679
C	-3.174853	-1.557495	2.946531
H	-2.334581	-2.014162	2.414850
H	-2.784347	-0.726595	3.546336
H	-3.581241	-2.305264	3.636234
C	-4.851405	0.699917	0.190187
H	-5.544414	1.160476	0.904939
H	-4.405672	1.516822	-0.388485
C	-5.628268	-0.221309	-0.755898
H	-4.932335	-0.715128	-1.447625
H	-6.111867	-1.023298	-0.184174
C	-6.690643	0.529806	-1.564960
H	-6.206421	1.331834	-2.138581
H	-7.387385	1.024434	-0.874543
C	-7.470860	-0.380952	-2.515186
H	-8.223099	0.179553	-3.081338
H	-6.801660	-0.863980	-3.237271
H	-7.990643	-1.174159	-1.964596
H	-0.792709	1.842394	-0.196166
H	3.829410	0.386132	-1.824653
O	4.674512	-0.400334	-0.007301
H	3.933734	-1.027359	-0.171414
O	2.837812	-0.320959	-2.817743
H	2.623732	-1.040538	-2.183359
H	2.081538	0.295353	-2.655675
H	3.942120	2.065022	0.400069
C	5.927238	0.434172	-1.915371
H	6.001512	1.282373	-2.599939
H	5.798685	-0.484996	-2.501719
O	7.098283	0.393301	-1.132073
H	6.963697	-0.324261	-0.492993

IM5a

Free Energy = -1792.7768313 Hartree

Energy = -1793.2829417 Hartree

Sn	0.312634	1.172255	-1.447849
O	-2.672842	1.105438	-0.212950
C	-1.814187	0.788469	0.645021
O	-0.572607	0.571219	0.352732
C	-2.178983	0.636849	2.110196
H	-3.194673	1.031100	2.224570
C	-2.182955	-0.857643	2.500272
H	-2.376463	-0.910133	3.578020
H	-1.177845	-1.264937	2.339439
C	-3.219124	-1.694484	1.748037
H	-4.221973	-1.269844	1.853477
H	-2.996803	-1.753767	0.678593
H	-3.238448	-2.718956	2.134605
C	-1.218296	1.448023	2.996711

H	-1.555823	1.343912	4.035228
H	-0.220504	0.998995	2.938129
C	-1.134287	2.932474	2.629805
H	-0.750361	3.035404	1.605728
H	-2.142805	3.369093	2.628387
C	-0.233345	3.732567	3.575719
H	0.763278	3.272796	3.595917
H	-0.626975	3.658432	4.598482
C	-0.108740	5.204331	3.177026
H	0.538259	5.754472	3.869285
H	0.317213	5.304876	2.171475
H	-1.087981	5.697950	3.172136
C	-5.940484	-1.076778	-1.502000
H	-6.328852	-1.289877	-2.492339
C	-5.655530	0.178750	-1.140185
O	-1.796383	-2.760230	-1.253814
C	-0.451355	-4.157886	0.942697
C	-0.218526	-5.191518	1.849838
C	1.073959	-5.677990	2.045829
C	2.130062	-5.128351	1.316767
C	1.927528	-4.098464	0.392209
C	0.614891	-3.607754	0.219353
H	-1.451608	-3.781195	0.784096
H	-1.053321	-5.609007	2.405328
H	1.260008	-6.480400	2.753415
H	3.138482	-5.509456	1.454199
C	3.078783	-3.542195	-0.406194
H	3.985830	-4.124849	-0.229264
H	2.865371	-3.557756	-1.481505
H	3.298081	-2.502355	-0.140420
N	0.434030	-2.534098	-0.682348
C	-0.718890	-2.188074	-1.304273
O	-0.548127	-1.065147	-2.079170
O	1.941991	-0.130645	-0.869586
C	2.491031	0.716829	-0.054291
O	1.949725	1.851599	0.045363
C	3.746973	0.322471	0.681343
H	3.545918	-0.675083	1.092025
C	4.072725	1.275234	1.839077
H	5.075983	1.025762	2.203950
H	4.115721	2.303295	1.466487
C	3.067292	1.184036	2.989154
H	2.062626	1.456132	2.653430
H	3.023455	0.166671	3.395697
H	3.342268	1.859187	3.806568
C	4.897386	0.166212	-0.346156
H	5.776482	-0.194857	0.200405
H	4.622174	-0.619171	-1.058961
C	5.254989	1.443660	-1.112009
H	4.371059	1.816747	-1.648088
H	5.543592	2.234227	-0.408207
C	6.389833	1.225293	-2.117956
H	6.100937	0.431657	-2.820260
H	7.277144	0.856489	-1.585827
C	6.747995	2.493323	-2.895575
H	7.560546	2.310930	-3.607531
H	5.885909	2.865928	-3.461672
H	7.070495	3.293914	-2.219228
H	1.217590	-1.900117	-0.818384
H	-3.555871	-0.758397	-2.492467
O	-5.279488	0.490898	0.144839
H	-4.367823	0.873236	0.123765
O	-2.840860	-0.117719	-2.646857
H	-2.828684	0.419799	-1.820891
H	-1.477261	-0.817288	-2.434821
H	-5.819364	-1.900599	-0.805615
C	-5.777170	1.385530	-2.038900
H	-6.214396	1.106593	-3.001088
H	-4.772770	1.794635	-2.238202
O	-6.615138	2.377071	-1.450395
H	-6.347308	2.424373	-0.519578

IM6

Free Energy = -1716.325678 Hartree

Energy = -1716.8005861 Hartree

Sn	-0.055085	-1.481066	-1.412949
O	0.837315	-2.804563	1.083477
C	0.479916	-1.657315	1.419061
O	0.164220	-0.752033	0.538382
C	0.339978	-1.239849	2.871008
H	0.593946	-2.123425	3.466480
C	1.317366	-0.098827	3.213548
H	1.140989	0.186572	4.257558
H	1.064508	0.773727	2.601351
C	2.789574	-0.464101	3.018086
H	3.059397	-1.346565	3.610224
H	3.022340	-0.680910	1.971348
H	3.438964	0.359553	3.333733
C	-1.118881	-0.828262	3.159725
H	-1.211608	-0.668127	4.241138
H	-1.309660	0.136561	2.678030
C	-2.172046	-1.837162	2.691592

H	-2.111282	-1.942460	1.600833
H	-1.957052	-2.827482	3.116416
C	-3.599764	-1.420021	3.059421
H	-3.785399	-0.407275	2.677356
H	-3.691055	-1.356952	4.152202
C	-4.660886	-2.373465	2.506245
H	-5.672248	-2.049344	2.775842
H	-4.609097	-2.426596	1.412431
H	-4.521759	-3.389988	2.893453
C	4.341301	-2.371739	-1.584403
H	4.237248	-2.524697	-2.656864
C	3.413693	-2.944749	-0.791893
O	3.657702	0.843102	-0.233873
C	2.413778	3.109747	1.197394
C	2.454343	4.308077	1.909783
C	1.815914	5.443062	1.408635
C	1.147012	5.372806	0.185186
C	1.101426	4.188408	-0.558506
C	1.739985	3.048675	-0.027907
H	2.903366	2.224375	1.580299
H	2.978771	4.346412	2.860014
H	1.839685	6.376988	1.962178
H	0.654893	6.255647	-0.213854
C	0.393714	4.131672	-1.887732
H	0.048139	5.125100	-2.183399
H	1.053771	3.747612	-2.674250
H	-0.481012	3.471457	-1.855743
N	1.638674	1.839222	-0.756553
C	2.565957	0.855114	-0.773300
O	2.135548	-0.203052	-1.550912
O	-0.756066	0.573119	-1.767053
C	-1.941629	0.343045	-1.304809
O	-2.207209	-0.847579	-0.961704
C	-2.930778	1.468906	-1.142625
H	-2.509432	2.324120	-1.680404
C	-3.022270	1.842882	0.356221
H	-3.816886	2.591387	0.457936
H	-3.340022	0.963586	0.924290
C	-1.714500	2.386427	0.932807
H	-0.909037	1.649919	0.862793
H	-1.394042	3.288466	0.403063
H	-1.836314	2.646037	1.989693
C	-4.307485	1.142649	-1.767943
H	-4.862114	2.088446	-1.814486
H	-4.153796	0.825519	-2.807615
C	-5.163015	0.098989	-1.040634
H	-4.608239	-0.841699	-0.967670
H	-5.356279	0.427830	-0.012021
C	-6.503706	-0.149945	-1.739232
H	-6.320307	-0.480354	-2.770855
H	-7.057818	0.795847	-1.814230
C	-7.360264	-1.189870	-1.013275
H	-8.315228	-1.354084	-1.524842
H	-6.842761	-2.154933	-0.954594
H	-7.581631	-0.872134	0.012758
H	0.768783	1.657159	-1.252457
H	2.861068	-0.881476	-1.542223
O	3.460504	-2.910411	0.554500
H	2.549290	-3.049101	0.897050
C	5.568396	-1.661432	-1.085202
H	5.691218	-0.706721	-1.616245
H	5.462125	-1.432346	-0.023732
O	6.758248	-2.456677	-1.203280
H	6.876734	-2.648831	-2.144936
H	2.567504	-3.475644	-1.228548

IM6a

Free Energy = -1716.330546 Hartree

Energy = -1716.7998033 Hartree

Sn	0.170238	-1.549671	-1.157443
O	-0.043276	-2.341451	1.112173
C	0.346354	-1.197002	1.476981
O	0.680332	-0.344975	0.568677
C	0.349819	-0.779401	2.929660
H	0.404391	-1.704417	3.514887
C	1.537023	0.132126	3.278456
H	1.423932	0.437113	4.325865
H	1.466817	1.043657	2.674921
C	2.905477	-0.518047	3.072365
H	2.998222	-1.440129	3.658508
H	3.071560	-0.771246	2.022585
H	3.707619	0.158547	3.387888
C	-0.993346	-0.075649	3.249387
H	-0.983550	0.159472	4.320931
H	-1.017353	0.882752	2.718343
C	-2.254497	-0.876024	2.912183
H	-2.308416	-1.041756	1.830126
H	-2.194895	-1.870409	3.375565
C	-3.536440	-0.175248	3.374111
H	-3.578677	0.827951	2.929129
H	-3.500218	-0.026476	4.461914
C	-4.801860	-0.951244	3.002428

H	-5.706905	-0.425509	3.326735
H	-4.870445	-1.095596	1.918172
H	-4.807954	-1.944200	3.467913
C	4.463063	-2.626541	-0.945002
H	4.900506	-1.810123	-0.380213
H	4.932769	-2.931572	-1.873474
C	3.434634	-3.339398	-0.453043
C	2.874044	-4.580282	-1.114401
H	3.444276	-5.451832	-0.767635
H	2.980002	-4.511418	-2.202120
O	1.502648	-4.692001	-0.725387
H	1.290810	-5.626364	-0.593241
O	4.044824	0.719823	-0.302828
C	2.848134	3.165462	0.793523
C	2.837649	4.406156	1.431452
C	2.167608	5.486599	0.857265
C	1.516591	5.317672	-0.366533
C	1.519076	4.089335	-1.035370
C	2.190049	3.003276	-0.432545
H	3.366732	2.324065	1.232338
H	3.349635	4.519882	2.382627
H	2.153475	6.452820	1.352681
H	0.998608	6.156277	-0.824254
C	0.826115	3.927579	-2.363700
H	0.426561	4.884230	-2.708703
H	1.514384	3.546142	-3.127479
H	-0.007396	3.218049	-2.306069
N	2.134109	1.757747	-1.095679
C	2.999928	0.723983	-0.933096
O	2.562681	-0.365374	-1.638189
O	-0.442982	0.562838	-1.899844
C	-1.582850	0.430237	-1.343019
O	-1.832913	-0.678100	-0.752071
C	-2.595447	1.551009	-1.347914
H	-2.175051	2.331117	-1.990590
C	-2.726825	2.122814	0.080793
H	-3.533531	2.865470	0.070118
H	-3.040211	1.323177	0.757992
C	-1.435453	2.760953	0.595060
H	-0.613896	2.038542	0.621385
H	-1.125946	3.594607	-0.042777
H	-1.569712	3.149540	1.610052
C	-3.949810	1.116798	-1.957524
H	-4.513745	2.036179	-2.160628
H	-3.760557	0.651597	-2.933945
C	-4.816411	0.180071	-1.108659
H	-4.247394	-0.721931	-0.861265
H	-5.061595	0.665393	-0.155762
C	-6.118683	-0.211361	-1.815073
H	-5.880013	-0.711332	-2.763816
H	-6.677578	0.696821	-2.079809
C	-7.002174	-1.125337	-0.963006
H	-7.922358	-1.401463	-1.490067
H	-6.476278	-2.051878	-0.702953
H	-7.290014	-0.634504	-0.025603
H	1.273459	1.539698	-1.591202
H	3.210385	-1.098038	-1.487974
O	2.839656	-3.020926	0.717859
H	2.000515	-3.523434	0.759022

IM7

Free Energy = -268.3689032 Hartree

Energy = -268.4609239 Hartree

C	1.800072	-0.565691	-0.143973
H	2.701551	0.032842	-0.225495
H	1.888144	-1.645409	-0.185099
C	0.603067	0.002971	0.034846
C	-0.680608	-0.769490	0.244063
H	-0.848697	-0.908555	1.320870
H	-0.615291	-1.759038	-0.222100
O	-1.739697	0.013093	-0.324145
H	-2.538273	-0.131283	0.201905
O	0.439668	1.350704	0.108687
H	-0.522393	1.494327	0.023966

IM7a

Free Energy = -268.3612295 Hartree

Energy = -268.4559897 Hartree

C	-0.025356	0.811400	0.133037
H	0.281696	1.851713	0.051085
C	-1.306365	0.528678	-0.129589
O	-1.813069	-0.736155	-0.044777
H	-2.749077	-0.715426	-0.287617
C	1.015817	-0.197021	0.522177
H	1.458553	0.074983	1.494179
H	0.563154	-1.185456	0.635754
O	2.050476	-0.352530	-0.461454
H	2.454961	0.518753	-0.583722
H	-2.013118	1.306571	-0.413585

3/3’

Free Energy = -515.5695065 Hartree

Energy = -515.7173865 Hartree

O	2.409353	-1.439053	-0.000129
C	-0.504698	-1.368685	0.000047
C	-1.833946	-1.792639	0.000031
C	-2.873603	-0.863954	0.000007
C	-2.568516	0.498696	-0.000012
C	-1.248726	0.958754	-0.000009
C	-0.206820	0.001566	0.000031
H	0.304603	-2.084836	0.000103
H	-2.048883	-2.857492	0.000023
H	-3.908739	-1.191755	-0.000002
H	-3.370450	1.232242	-0.000053
C	-0.951922	2.437741	-0.000028
H	-1.879560	3.014494	-0.000209
H	-0.373508	2.738276	0.883424
H	-0.373262	2.738221	-0.883335
N	1.115599	0.488064	0.000007
C	2.278917	-0.225049	-0.000020
O	3.332142	0.631992	0.000060
H	1.231891	1.491938	0.000046
H	4.132648	0.080376	0.000238

IM1A

Free Energy = -1755.6442345 Hartree

Energy = -1756.1169601 Hartree

Sn	-0.097366	-0.926888	-1.910759
O	-0.107626	-2.827715	0.239977
C	0.139516	-1.748090	0.813743
O	0.362695	-0.661702	0.134881
C	0.087897	-1.615455	2.326618
H	0.274027	-2.618617	2.727502
C	1.111412	-0.619679	2.896050
H	0.896249	-0.500287	3.965124
H	0.940573	0.356337	2.431111
C	2.573865	-1.024889	2.716280
H	2.779187	-1.988362	3.196475
H	2.844789	-1.111652	1.659438
H	3.237740	-0.283890	3.174617
C	-1.344975	-1.180027	2.730610
H	-1.393877	-1.215482	3.826187
H	-1.474990	-0.130344	2.446304
C	-2.493664	-2.001001	2.139462
H	-2.494011	-1.896849	1.049025
H	-2.339813	-3.067631	2.352200
C	-3.859713	-1.560298	2.676382
H	-3.985108	-0.484238	2.494956
H	-3.885286	-1.691751	3.766769
C	-5.023123	-2.321530	2.037366
H	-5.989201	-1.982512	2.427437
H	-5.034156	-2.180053	0.950494
H	-4.944566	-3.398346	2.229405
C	4.589415	-0.403176	-1.505067
H	4.802050	0.030693	-2.486360
C	4.088203	-1.822009	-1.689571
O	3.720064	0.512601	-0.775724
C	3.133640	2.324944	1.399878
C	3.513931	3.244462	2.377037
C	3.094906	4.572293	2.288563
C	2.303464	4.976403	1.211681
C	1.919930	4.079671	0.208669
C	2.344886	2.740217	0.323296
H	3.442119	1.291731	1.472186
H	4.126997	2.914660	3.210400
H	3.382285	5.290575	3.050470
H	1.980732	6.011043	1.135417
C	1.088806	4.531098	-0.964775
H	0.915927	5.608880	-0.921897
H	1.583865	4.297646	-1.914436
H	0.109620	4.037777	-0.986248
N	1.889333	1.834790	-0.669604
C	2.500206	0.773590	-1.219264
O	1.940479	0.097236	-2.119391
O	-0.709952	1.184610	-1.710094
C	-1.855617	0.953329	-1.149746
O	-2.213034	-0.245688	-1.004885
C	-2.689035	2.118394	-0.662759
H	-2.215342	3.019334	-1.066773
C	-2.615135	2.189266	0.879308
H	-3.300298	2.979560	1.208816
H	-2.990461	1.250214	1.297047
C	-1.206866	2.463663	1.410157
H	-0.504919	1.684326	1.100020
H	-0.827398	3.423604	1.046723
H	-1.202803	2.496627	2.504705
C	-4.140129	2.065982	-1.194450
H	-4.585856	3.049941	-0.999198
H	-4.109053	1.955252	-2.286413
C	-5.048795	0.982164	-0.602902
H	-4.592807	-0.000517	-0.759036
H	-5.131188	1.118665	0.482669
C	-6.454842	1.002289	-1.211247
H	-6.381803	0.862901	-2.298601

H	-6.903807	1.993628	-1.059423
C	-7.371004	-0.070929	-0.618500
H	-8.372385	-0.035460	-1.061843
H	-6.965106	-1.074641	-0.790949
H	-7.480935	0.058998	0.464737
H	0.933325	1.950625	-1.007851
H	3.220695	-1.837054	-2.354583
O	3.770247	-2.412198	-0.443534
H	4.903389	-2.371005	-2.191015
H	5.499225	-0.391548	-0.903793
C	2.964143	-3.574422	-0.613402
H	3.464575	-4.302792	-1.270445
H	2.010780	-3.300210	-1.087140
C	2.674157	-4.185411	0.756702
H	3.523146	-4.788147	1.097944
H	2.542274	-3.368710	1.474859
O	1.537211	-5.032235	0.713430
H	0.781013	-4.426401	0.590135

TS1A

Free Energy = -1755.5728408 Hartree

Energy = -1756.0502774 Hartree

Sn	0.150402	-0.970509	-1.784579
O	-0.122367	-2.820062	0.367664
C	0.141875	-1.750837	0.954287
O	0.384806	-0.663153	0.288224
C	0.135916	-1.629588	2.466997
H	0.270967	-2.644807	2.857525
C	1.256913	-0.712383	2.983408
H	1.154382	-0.637553	4.072964
H	1.093564	0.292622	2.580354
C	2.669162	-1.182108	2.631619
H	2.872453	-2.175258	3.048356
H	2.821023	-1.237047	1.549433
H	3.419924	-0.494208	3.036320
C	-1.247893	-1.104188	2.922750
H	-1.269212	-1.150644	4.018849
H	-1.320097	-0.044761	2.652767
C	-2.457178	-1.849700	2.350740
H	-2.482421	-1.722689	1.261960
H	-2.352015	-2.927535	2.535025
C	-3.783690	-1.357026	2.938313
H	-3.862324	-0.271977	2.787415
H	-3.783361	-1.515211	4.025398
C	-4.999857	-2.046918	2.316391
H	-5.937556	-1.669782	2.739558
H	-5.032494	-1.882049	1.233529
H	-4.969168	-3.130065	2.484850
C	5.076508	-0.795281	-1.182018
H	5.447066	-0.159690	-1.976206
C	4.196209	-1.824138	-1.486577
O	3.861451	0.982393	-0.480798
C	2.801623	2.927070	1.442456
C	2.977681	4.004927	2.309496
C	2.400877	5.241526	2.015146
C	1.658932	5.393277	0.842149
C	1.481181	4.333206	-0.053985
C	2.058388	3.087177	0.266578
H	3.237375	1.961577	1.665625
H	3.555629	3.870915	3.219284
H	2.528432	6.082419	2.690406
H	1.213186	6.355505	0.604331
C	0.699365	4.514203	-1.329500
H	0.416222	5.561094	-1.463222
H	1.284776	4.198870	-2.200958
H	-0.219072	3.915682	-1.333412
N	1.816280	2.001652	-0.605832
C	2.683141	0.994410	-0.893797
O	2.212693	0.040342	-1.683549
O	-0.625678	1.082140	-1.727756
C	-1.796226	0.791745	-1.244937
O	-2.087506	-0.421715	-1.090489
C	-2.727991	1.913755	-0.845952
H	-2.294111	2.831913	-1.254929
C	-2.736063	2.035272	0.695591
H	-3.485105	2.790115	0.963365
H	-3.073335	1.087541	1.125615
C	-1.377167	2.414562	1.286902
H	-0.618396	1.659324	1.062810
H	-1.026378	3.372448	0.890774
H	-1.440765	2.508059	2.376134
C	-4.143492	1.749389	-1.445797
H	-4.657588	2.710170	-1.313458
H	-4.048823	1.599504	-2.529306
C	-5.014850	0.634566	-0.855785
H	-4.490896	-0.322409	-0.943441
H	-5.166821	0.810688	0.216330
C	-6.382714	0.539043	-1.539564
H	-6.239246	0.358280	-2.613719
H	-6.899217	1.505467	-1.458307
C	-7.264393	-0.563744	-0.948727
H	-8.237696	-0.612528	-1.449656

H	-6.787963	-1.546000	-1.050426
H	-7.446909	-0.393717	0.118964
H	0.886343	1.918840	-1.013638
H	3.267639	-0.971663	-1.616725
O	3.936020	-2.740115	-0.478258
H	4.208636	-2.215980	-2.511667
H	5.484550	-0.666839	-0.187405
C	2.862229	-3.639876	-0.760692
H	3.116172	-4.286417	-1.612383
H	1.952993	-3.086261	-1.019417
C	2.593544	-4.459489	0.499433
H	3.391013	-5.195570	0.649767
H	2.606593	-3.778338	1.361154
O	1.369339	-5.161729	0.396263
H	0.675724	-4.476075	0.449267

IM2A

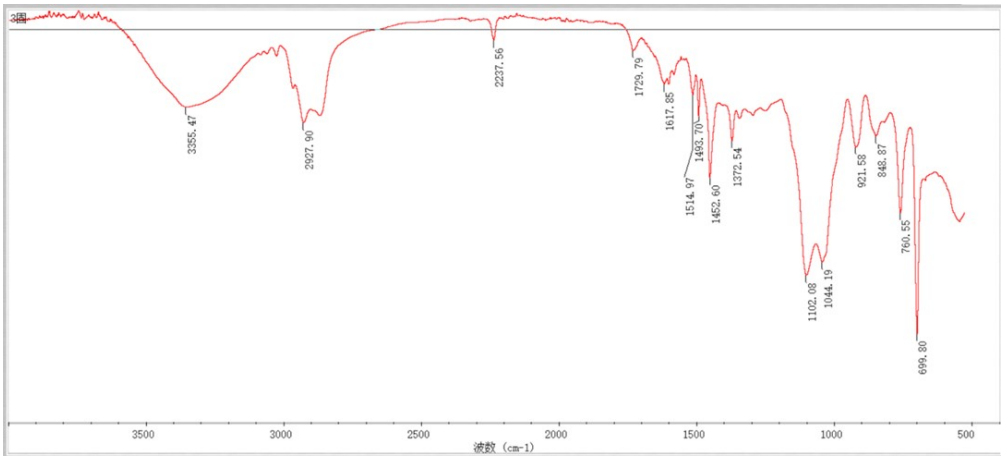
Free Energy = -1755.63238 Hartree

Energy = -1756.1099076 Hartree

Sn	0.201831	-1.097791	-1.657976
O	0.088698	-2.477729	0.521196
C	0.384487	-1.378334	1.061666
O	0.622939	-0.356091	0.308825
C	0.382961	-1.204520	2.563687
H	0.629804	-2.187327	2.982472
C	1.390977	-0.150657	3.048062
H	1.261712	-0.046350	4.131998
H	1.124608	0.814889	2.605251
C	2.852794	-0.471834	2.736416
H	3.151217	-1.430310	3.175542
H	3.034680	-0.515654	1.658503
H	3.512892	0.299896	3.147344
C	-1.051038	-0.820426	3.016734
H	-1.040874	-0.799712	4.113387
H	-1.250371	0.205156	2.686651
C	-2.179899	-1.733665	2.531539
H	-2.239674	-1.698272	1.438106
H	-1.955223	-2.775985	2.795594
C	-3.540445	-1.338498	3.115358
H	-3.739493	-0.284332	2.879478
H	-3.502699	-1.405244	4.211136
C	-4.685310	-2.203974	2.584251
H	-5.650146	-1.897289	3.003159
H	-4.757207	-2.132242	1.492921
H	-4.532179	-3.260198	2.836003
C	4.730932	-1.540292	-2.314908
H	4.739927	-1.228020	-3.353376
C	3.983292	-2.594272	-1.948760
O	3.845630	1.243370	-0.350717
C	2.496750	3.243818	1.333660
C	2.428232	4.302112	2.239873
C	1.675803	5.437695	1.938700
C	1.000991	5.510099	0.718428
C	1.060260	4.470159	-0.215074
C	1.814917	3.324111	0.113071
H	3.077950	2.360586	1.560547
H	2.959296	4.229270	3.184474
H	1.616224	6.261940	2.643142
H	0.418928	6.394453	0.473272
C	0.338676	4.569516	-1.534504
H	-0.128283	5.551010	-1.644993
H	1.024712	4.417071	-2.376056
H	-0.450058	3.813179	-1.626313
N	1.818687	2.259024	-0.815617
C	2.772240	1.300833	-0.924260
O	2.385934	0.355496	-1.846087
O	-0.626211	0.989224	-1.860592
C	-1.737052	0.643130	-1.319555
O	-1.877964	-0.586133	-1.009608
C	-2.812536	1.657899	-1.023881
H	-2.477565	2.594999	-1.479902
C	-2.900591	1.868428	0.504732
H	-3.760011	2.520625	0.699870
H	-3.114129	0.909140	0.985190
C	-1.633095	2.479685	1.103573
H	-0.759211	1.845322	0.927481
H	-1.425601	3.461984	0.668855
H	-1.736687	2.609077	2.185849
C	-4.169068	1.277326	-1.663559
H	-4.802140	2.172164	-1.610994
H	-4.009035	1.077067	-2.731069
C	-4.920111	0.099255	-1.033088
H	-4.285807	-0.792890	-1.050809
H	-5.126791	0.313644	0.022772
C	-6.243316	-0.196553	-1.746928
H	-6.043369	-0.416209	-2.804629
H	-6.872999	0.703716	-1.734969
C	-7.006690	-1.363927	-1.116946
H	-7.948530	-1.558949	-1.641744
H	-6.412140	-2.284825	-1.145698
H	-7.246428	-1.157794	-0.067034
H	0.963579	2.099380	-1.341443

H	3.134797	-0.286339	-1.940510
O	4.000249	-3.092796	-0.695991
H	3.325369	-3.101846	-2.654667
H	5.390332	-1.042409	-1.611326
C	2.922588	-3.992810	-0.368447
H	3.142282	-4.994439	-0.756941
H	1.993659	-3.635264	-0.823881
C	2.766109	-3.995009	1.149830
H	3.588010	-4.546724	1.618551
H	2.826471	-2.956107	1.497965
O	1.553766	-4.616848	1.536891
H	0.846394	-4.007146	1.24960

Figure S7 FTIR spectrum of the middle solid isolated after kilogram-scale glycerolysis and phase separation



A pronounced **C≡N band at ~2237 cm⁻¹**, together with **aromatic C=C** bands (≈1600/1514/1462 cm⁻¹), out-of-plane **Ar–H** vibrations (≈760/698 cm⁻¹), and **polyether C–O–C** features (≈1102/1014 cm⁻¹), is consistent with a **SAN/PPG polymer-polyol (POP)–enriched residue**. Only a **weak** carbonyl feature is observed near **~1729 cm⁻¹**, suggesting minor ester/urethane-type impurities but not a dominant polyurethane character in this phase.

Note. This phase-specific FTIR identifies functional groups **enriched in the insoluble residue** and **should not be interpreted as a measure of overall conversion**; quantitative depolymerization is reflected by diamine yields and phase distributions reported in the main text.

Figure S8 GPC chromatograms of the upper polyether-polyol-rich phase and the lower diamine-rich phase obtained from crude-glycerol glycolysis of waste car seat cushions

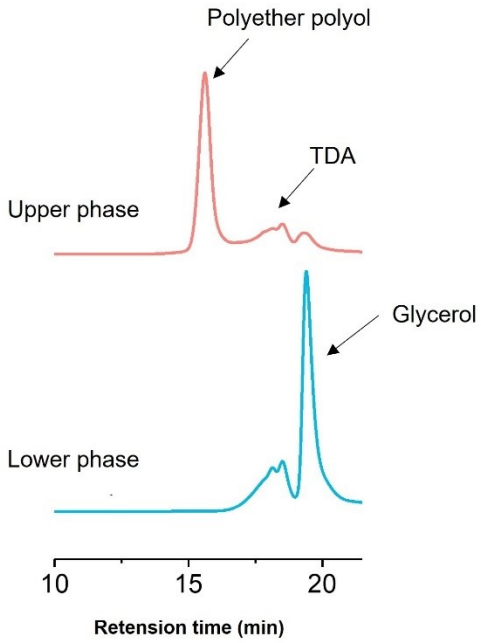


Table S3 Physicochemical properties of recycled polyether-polyol-rich upper phases

Sample	OH number (mg KOH g^{-1})	Water content (wt%)	Gardner colour	Note
Upper phase from crude glycerol	104.8	0.38	15.8	Representative upper phase from crude-glycerol kilogram-scale glycolysis.
Upper phase from pure glycerol	72.4	0.12	9.2	Upper phase obtained under otherwise similar conditions using pure glycerol.

Table S4 Effect of 2-pyrrolidone on foam dissolution and product yields in crude-glycerol glycolysis of waste car seat cushions

2-Pyrrolidone	Dissolution time	Extra time	Total time	Aniline yield (%)	Polyol yield (%)	Comment
Absent	1–1.5 h	5 h	6–6.5 h	15.9	47.2	Reference run without 2-pyrrolidone; high TDA yield and typical polyether-polyol recovery for crude-glycerol kilogram-scale glycolysis.
Present	< 30 min	5 h	ca. 5.5 h	16.3	46.8	TDA and polyether-polyol yields essentially identical to the run without 2-pyrrolidone; main effect of 2-pyrrolidone is to shorten the dissolution/feeding period.

Table S5 Comparison of the present glycerol-enabled glycolysis with representative PU deconstruction and diamine-/polyol-recovery methods

Method / reference	Reagents & conditions	Main products	Diamine recovery	Green / waste aspects
Dimethyl H-phosphonate degradation (Ref. [6])	Flexible TDI-based PU foams; dimethyl H-phosphonate (DMP) with catalysts in an organic medium; ca. 160–190°C, sealed reactor, several hours	Degraded polyol-like fractions, phosphonate-modified products	Not targeted; aromatic diamines not reported as isolated products	Uses organophosphorus reagent; generates P-containing organic waste; route is polyol-centred rather than diamine-centred
Adipic-acid acidolysis (Ref. [15])	Flexible PU foams; adipic acid; mostly solvent-free; microwave heating at ca. 180–220°C, typically < 1 h	Recycled polyols with controlled OH numbers and molar-mass distribution	Aromatic diamines mainly remain as minor impurities in polyols; not isolated as pure monomers	Requires relatively high loading of dicarboxylic acid; neutralisation gives salt-containing aqueous waste; focuses on polyol recovery
Multistage glycolysis–hydrolysis (Ref. [23])	Model PUs / dicarbamates; excess glycol for split-phase glycolysis followed by aqueous hydrolysis; high-temperature glycolysis plus separate hydrolysis step	Polyols from upper glycolysis phase; amines from hydrolysis of carbamate intermediates	Demonstrated amine yields only moderate (for selected model systems)	Multistep process; more complex operation and waste management; generates aqueous streams containing salts and organics
Fast maleic-acid acidolysis (Ref. [25])	TDI-based flexible PU foams; maleic acid under (nearly) solvent-free conditions; < 200°C, typically < 10 min	Recycled polyols with nearly quantitative polyol recovery and good re-foaming performance	Aromatic diamines not obtained as isolated monomers; isocyanate segment converted to other species	High acid usage; neutralisation produces significant salt-containing aqueous waste; polyol-centred, limited diamine valorisation
tert-Amyl alcohol-mediated deconstruction (Ref. [28])	Flexible / rigid PU foams; tert-amyl alcohol (t-AmOH) as solvent and reagent; base catalyst; ca. 220–230°C, several hours, sealed reactor	Polyols, aniline/aromatic diamines and diisocyanate-type products	High overall yield of aniline / related diamines reported for selected systems	Requires large excess of high-boiling organic solvent (t-AmOH); solvent recovery and handling needed; higher operating temperature
This work: glycerol-enabled glycolysis	Waste mattresses and car seat cushions (TDI-based flexible PU foams); glycerol or crude glycerol as both reagent and reaction medium; stannous octoate catalyst; 200°C, 1 atm, 3–5 h, stirred batch	TDA-rich lower phase and polyether-polyol-rich upper phase, plus small solid residue	TDA yield up to ca. 98–99% for TDI-based flexible foams; diamine-rich fraction isolated by simple acidification and crystallisation	Uses low-value crude glycerol; no strong mineral acids and no additional organic solvent during depolymerisation; simple phase separation; relatively low estimated energy demand (~0.5–1.0 kWh per kg PU under lab conditions); simultaneous valorisation of isocyanate and polyether segments