

## Supplementary Information

### Lewis Pair Polymerization by Classical and Frustrated Lewis Pairs: Acid, Base and Monomer Scope and Polymerization Mechanism

Yuetao Zhang,<sup>†</sup> Garret M. Miyake,<sup>†</sup> Mallory G. John,<sup>†</sup> Laura Falivene,<sup>‡</sup> Lucia Caporaso,<sup>‡</sup> Luigi Cavallo,<sup>\*,§</sup> and Eugene Y.-X. Chen<sup>\*,†</sup>

#### Cartesian Coordinates with BP86 and M06 solvent phase energies (in a.u.).

Al(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub>			MMA			Al(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> -MMA					
E <sub>BP86</sub> = -2426.735258			E <sub>BP86</sub> = -345.906991			E <sub>BP86</sub> = -2772.683230					
E <sub>M06</sub> = -2425.720189			E <sub>M06</sub> = -345.678099			E <sub>M06</sub> = -2771.459124					
Al	-0.002935	-0.000305	0.000580	C	-0.979046	-0.679498	0.000000	Al	-0.013571	0.032652	0.126754
C	0.871598	1.761106	0.000141	C	0.000000	0.466041	0.000000	C	-1.578685	-1.173346	-0.235239
C	2.139463	4.300204	-0.000262	C	-2.288764	-0.341239	0.000000	C	-2.857963	-0.787838	0.196569
F	2.736241	5.493717	-0.001060	C	-0.489119	-2.114546	0.000000	C	-4.021804	-1.533682	-0.058173
C	0.604313	2.713995	-0.994040	H	-3.080439	-1.108016	0.000000	C	-3.906566	-2.742265	-0.771723
C	1.218118	3.978125	-1.017687	H	-2.582754	0.719953	0.000000	C	-2.644329	-3.181551	-1.212663
F	-0.268063	2.410393	-1.982238	H	0.613722	-2.169228	0.000000	C	-1.514777	-2.391741	-0.928009
F	0.951309	4.867119	-1.980674	H	-0.860140	-2.660142	0.892972	C	-0.344487	1.985817	-0.186528
C	-1.965518	-0.124670	0.001279	H	-0.860140	-2.660142	-0.892972	C	0.414842	2.968502	0.463533
C	-4.797829	-0.303386	0.000431	O	1.293676	0.034126	0.000000	C	0.233677	4.349833	0.277652
C	-2.655237	-0.835148	-0.992492	O	-0.297382	1.650312	0.000000	C	-0.757462	4.781627	-0.624000
C	-2.739532	0.493425	0.994745	C	2.284827	1.071323	0.000000	C	-1.540954	3.835822	-1.311544
C	-4.142952	0.420264	1.017862	H	3.264546	0.559327	0.000000	C	-1.314451	2.465472	-1.081508
C	-4.056553	-0.939358	-1.016380	H	2.183732	1.715130	-0.898054	C	1.791347	-0.524423	-0.546457
F	-1.954258	-1.437701	-1.980134	H	2.183732	1.715130	0.898054	C	1.930906	-0.632175	-1.938099
F	-2.120623	1.179613	1.982586					C	3.136911	-0.963820	-2.578269
F	-4.858535	1.014112	1.979316					C	4.276777	-1.192514	-1.783226
F	-4.691249	-1.617909	-1.978605					C	4.191118	-1.086899	-0.382344
F	-6.129609	-0.387091	-0.000147					C	2.955208	-0.751016	0.201304
C	1.793797	2.120496	0.994385					F	2.936304	-0.645184	1.556239
C	2.434916	3.370979	1.018147					F	5.281498	-1.300563	0.370125
F	2.075144	1.240649	1.982706					F	5.442103	-1.507678	-2.359467
F	3.306727	3.691861	1.980506					F	3.223655	-1.057072	-3.912009
C	1.087171	-1.636981	0.000894					F	0.849813	-0.397856	-2.722934
C	2.664031	-3.996358	-0.001779					F	-2.536254	-4.340938	-1.877375
C	2.042896	-1.879054	-0.970666					F	-0.316592	-2.874030	-1.340051
C	0.945773	-2.614306	0.997325					F	-4.995769	-3.476926	-1.022280
C	1.714018	-3.791127	1.019683					F	-5.224310	-1.125179	0.371961
C	2.836520	-3.038721	-1.022060					F	-3.007455	0.360011	0.904832
F	2.206981	-0.971772	-1.987229					F	-2.080916	1.597787	-1.778305
F	0.045773	-2.421301	1.988677					F	-2.480178	4.251223	-2.172493
F	1.564946	-4.705640	1.984402					F	-0.953946	6.089299	-0.826362
F	3.737304	-3.249548	-1.988098					F	0.981882	5.250022	0.934050
F	3.405491	-5.105718	-0.002927					F	1.394961	2.595134	1.336341
								C	0.666606	-2.118943	3.300943
								C	0.335456	-0.684858	3.108139
								C	0.634910	-2.942067	2.224568
								C	1.009771	-2.577035	4.697611
								H	0.865744	-4.013219	2.336551
								H	0.383154	-2.591166	1.213067
								H	0.176534	-2.380922	5.403642
								H	1.233660	-3.660533	4.707367
								H	1.893718	-2.031872	5.089089
								O	0.287707	0.005257	4.237352
								O	0.098120	-0.115455	2.019225
								C	-0.046778	1.415663	4.157529
								H	0.079556	1.803188	5.182944
								H	0.625303	1.928554	3.443870
								H	-1.096644	1.529248	3.822180

<b>P<sup>t</sup>Bu<sub>3</sub></b>	<b>PPh<sub>3</sub></b>	<b>PMes<sub>3</sub></b>	<b>NHC<sup>mes</sup></b>	<b>PMe<sub>3</sub></b>
<b>E<sub>BP86</sub>=-815.0478372</b> <b>E<sub>M06</sub>=-814.6374144</b>	<b>E<sub>BP86</sub>=-1036.540481</b> <b>E<sub>M06</sub>=-1035.937736</b>	<b>E<sub>BP86</sub>=-1390.455731</b> <b>E<sub>M06</sub>=-1389.589633</b>	<b>E<sub>BP86</sub>=-924.4429528</b> <b>E<sub>M06</sub>=-923.7365278</b>	<b>E<sub>BP86</sub>=-461.1748458</b> <b>E<sub>M06</sub>=-461.0187089</b>
P -0.001166 -0.000936 -0.718723 C 1.698830 -0.667190 0.000575 C -0.270387 1.804216 0.001155 C -1.430019 -1.136350 0.001747 C 2.101797 -1.865189 -0.898736 C 2.793322 0.403003 -0.218579 C 1.722873 -1.102837 1.480071 C -1.745606 2.217596 -0.216324 C 0.096237 2.040805 1.481161 C 0.565326 2.750514 -0.899242 C -1.048203 -2.619668 -0.208726 C -1.821948 -0.932457 1.478814 C -2.662241 -0.889897 -0.906114 H -2.632216 -1.646035 1.753032 H -0.977046 -1.114688 2.171883 H -2.211320 0.085071 1.677141 H -3.463246 -1.617750 -0.646148 H -3.090438 0.123464 -0.795912 H -2.405120 -1.053163 -0.967919 H 3.130394 -2.196494 -0.630975 H 1.436118 -2.739826 -0.786570 H 2.106616 -1.576453 -1.969943 H 2.745957 -1.451655 1.748810 H 1.467153 -0.276318 2.171705 H 1.034989 -1.947092 1.685595 H 3.785763 -0.053606 -0.007021 H 2.814949 0.765171 -1.267210 H 2.690177 1.277219 0.453345 H -1.848567 3.304238 -0.000321 H -2.070524 2.058028 -1.265229 H -2.449629 1.687474 0.453777 H -0.117494 3.099457 1.754080 H -0.487283 1.399610 2.170375 H 1.171586 1.868258 1.685515 H -1.937356 -3.252144 0.009637 H -0.747166 -2.826041 -1.256834 H -0.236816 -2.961128 0.463396 H 0.334419 3.807450 -0.637788 H 1.655379 2.614707 -0.781432 H 0.318329 2.604012 -1.971166	P -0.001003 -0.000719 -1.223816 C 1.211286 -1.152415 -0.408549 C 0.391845 1.624089 -0.408518 C -1.605018 -0.472910 -0.408550 C -1.710899 -1.326772 0.711763 C -2.971991 -1.657435 1.240295 C -4.142549 -1.136399 0.662282 C -4.048541 -0.286578 -0.455219 C -2.791016 0.033112 -0.992443 H -0.799467 -1.737212 1.174269 H -3.038200 -2.326283 2.113776 H -5.129019 -1.396683 1.078242 H -4.961487 0.120589 -0.919007 H -2.725010 0.683286 -1.881229 C 1.369664 -2.431584 -0.993576 C 2.277021 -3.359221 -0.456259 C 3.057385 -3.015186 0.662720 C 2.920190 -1.741711 1.241748 C 2.001740 -0.816311 0.713295 H 0.774737 -2.699599 -1.883033 H 2.384337 -4.352470 -0.921324 H 3.777536 -3.738011 1.078450 H 3.531633 -1.463920 2.115613 H 1.899422 0.177655 1.176674 C -0.291727 2.140835 0.714727 C 0.052778 3.398517 1.242594 C 1.087081 4.153047 0.662272 C 1.773434 3.648366 -0.457429 C 1.420748 2.399655 -0.994745 H -1.100754 1.555035 1.179030 H -0.491185 3.789404 2.117809 H 1.354893 5.137622 1.077963 H 2.580706 4.236480 -0.923008 H 1.948318 2.018293 -1.8853	P 0.001017 -0.000188 0.781302 C -0.809594 1.563385 0.194100 C 1.760201 -0.080240 0.193992 C -0.948571 -1.483212 0.193432 C -1.958468 -1.509927 -0.817652 C -2.693950 -2.698579 -1.018500 C -2.468085 -3.871761 -0.277188 C -1.455087 -3.834252 0.698995 C -0.703125 -2.672288 0.957363 C -2.269890 -0.342448 -1.729114 H -3.466340 -2.705986 -1.806893 C -3.295183 -5.117492 -0.500553 H -1.242050 -4.740613 1.291525 C 0.362070 -2.729771 2.031634 C -1.961747 1.944377 0.959187 C -2.593443 3.175862 0.700849 C -2.121520 4.071577 -0.276709 C -0.993707 3.681045 -1.019626 C -0.330082 2.451043 -0.818413 C -2.541692 1.049771 2.034167 H -3.484149 3.444265 1.294499 C -2.788604 5.409803 -0.500627 H -0.616033 4.353037 -1.809655 C 0.835544 2.136764 -1.731119 C 2.289342 -0.944003 -0.814110 C 3.686531 -0.986074 -1.014581 C 4.588499 -0.201330 -0.275144 C 4.048269 0.660647 0.697947 C 2.665923 0.731221 0.954957 C 1.434324 -1.799456 -1.723601 H 4.080083 -1.653129 -1.801005 C 6.081178 -0.291672 -0.500246 H 4.725538 1.301476 1.288367 C 2.180318 1.686240 2.024670 H 3.032602 2.135296 2.572528 H 1.576362 2.515803 1.597547 H 1.517202 1.170540 2.752241 H 2.033300 -2.167706 -2.580542 H 1.011123 -2.684067 -1.203801 H 0.567142 -1.238324 -2.124600 H 6.570403 0.699623 -0.404845 H 6.559797 -0.960917 0.249062 H 6.320571 -0.699378 -1.503172 H -2.689540 -6.039204 -0.378877 H -4.130180 -5.180883 0.232475 H -3.747722 -5.133254 -1.512731 H 0.319701 -3.691436 2.580865 H 1.385101 -2.625399 1.610082 H 0.245713 -1.896725 2.757957 H -2.887923 -0.677684 -2.586034 H -2.824657 0.466312 -1.209412 H -1.350390 0.127649 -2.131060 H -2.580151 5.807051 -1.514840 H -3.889152 5.345837 -0.374928 H -2.423409 6.166790 0.228853 H -3.534765 1.564744 2.583682 H -2.959724 0.110111 1.612507 H -1.761016 0.736312 2.760367 H 0.849903 2.834905 -2.592094 H 1.814729 2.219423 -1.214973 H 0.785967 1.102971 -2.127268	C 0.000280 0.001301 -0.273717 N 1.069726 0.023475 0.598949 N -1.070036 -0.012307 0.598158 C 0.683780 0.024322 1.947581 C -0.685267 0.000260 1.947078 C 2.443476 0.035069 0.162024 C -2.443431 -0.031305 0.162046 C 2.985290 1.226933 -0.381524 C 4.333831 1.216228 -0.784120 C 5.144688 0.068449 -0.662424 C 4.566050 -1.097227 -0.126676 C 3.218610 -1.141687 0.288202 C 2.135871 2.465934 -0.537569 H 4.764529 2.139366 -1.208158 H 5.177622 -2.010881 -0.035671 C 2.620088 -2.420844 0.828633 C -2.979738 -1.227618 -0.378855 C -4.327285 -1.223454 -0.784839 C -5.143020 -0.078519 -0.669209 C -4.569195 -1.072994 -1.139686 C -3.222892 1.143571 0.278148 C -2.125311 -2.463799 -0.529877 H -4.752728 -2.149419 -1.207990 H -5.183322 2.420518 -0.057413 C -2.629097 2.428505 0.810042 C 6.587971 0.093341 -1.115962 C -6.592028 -1.118386 -1.102806 H 2.728849 3.307209 -0.946985 H 1.278189 2.266225 -1.213948 H 1.702186 2.787663 0.433426 H 3.295586 -3.280370 0.649683 H 2.431705 -2.365991 1.922557 H 1.642663 -2.637255 0.349942 H 7.116913 -0.844036 -0.851927 H 6.662098 0.221521 -2.217800 H 7.143478 0.938967 -0.657665 H -3.306994 3.284587 0.623803 H -2.442426 2.382159 1.904643 H -1.651531 2.644460 0.331445 H -1.268902 -2.263733 -1.207748 H -1.689563 -2.779039 0.442314 H -2.715261 -3.309405 -0.934735 H -7.057773 0.886757 -1.070230 H -6.695947 -0.508605 -2.137365 H -7.191029 -0.786943 -0.446687 H 1.402273 0.048482 2.774300 H -1.404473 -0.015859 2.773370	P -0.000020 -0.000062 -0.607927 C 0.325384 1.613968 0.281943 C -1.560650 -0.525138 0.282032 C 1.235157 -1.088738 0.282079 H 1.157381 -1.017974 1.389101 H 1.079982 -2.145514 -0.019594 H 2.263646 -0.803158 -0.022097 H -2.399090 0.134812 -0.023567 H -1.825547 -1.560317 -0.017895 H -1.461783 -0.487836 1.389035 H 1.319257 2.006091 -0.018406 H -0.434444 2.363213 -0.022974 H 0.301553 1.511054 1.388978

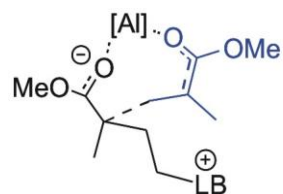




H	-5.133397	1.443922	2.705128	H	1.399199	-0.334730	1.342217	H	4.756214	-3.826672	-1.045274
H	-3.948290	3.725646	0.853033					H	4.945527	-5.305095	-0.063570
H	-3.072109	2.379537	1.615063					H	7.635210	4.904957	-1.627431
H	-2.946812	2.650936	-0.145078					H	5.910217	5.370741	-1.690188
H	-3.012721	-1.619738	-3.077917					H	6.823630	5.577643	-0.171006
H	-2.257286	-1.569842	-1.472004					H	4.272100	2.711373	2.813633
H	-3.828980	-2.420037	-1.709130					H	3.054195	1.897555	1.812438
								H	4.307660	0.930112	2.647700
								H	7.441918	-0.754032	-1.269077
								H	5.890422	-0.749653	-2.147893
								H	7.265635	0.223124	-2.755298
								H	2.476577	-1.281941	2.765477
								H	0.874127	-1.006335	1.993004
								H	0.991422	-2.006752	3.457331



H	1.967233	-3.960491	-1.181096	H	-0.460298	-5.817853	0.396733	C	-1.591581	-2.748902	3.462446
H	0.720304	-6.868611	-1.479585	H	1.195157	-6.970154	1.853503	C	-3.818227	-3.397148	-1.473404
H	1.014741	-6.056179	0.075582	H	2.896135	-5.635854	3.134553	C	-4.716641	-3.253973	-2.547486
H	-0.619789	-6.694856	-0.315275	H	2.938518	-3.131522	2.925190	C	-4.331774	-3.485631	-3.884407
H	-4.683943	-3.932127	-1.181763	H	1.296675	-1.966637	1.486537	C	-3.008136	-3.901188	-4.136130
H	-3.575153	-2.581719	-1.507709	C	-2.322336	-3.966618	-2.464920	C	-2.062967	-4.069539	-3.102586
H	-3.273912	-4.193764	-2.246883	C	-2.341090	-4.572805	-3.733037	C	-4.275126	-3.214621	-0.045771
H	-4.130000	-5.768358	0.356585	C	-1.154600	-5.075000	-4.298789	C	-5.753573	-2.954756	-2.334662
H	-2.762127	-6.219901	-0.690711	C	0.060940	-4.971125	-3.598871	C	-5.335796	-3.335006	-5.003578
H	-2.511054	-5.977235	1.072663	C	0.094339	-4.374108	-2.328454	C	-2.696463	-4.115146	-5.172022
H	-0.326460	-5.816762	-3.369911	H	-3.254112	-3.565913	-2.037182	C	-0.683939	-4.612235	-3.412390
H	-1.838882	-5.796456	-2.428871	H	-3.293398	-4.653677	-4.280141	H	0.110279	-4.190668	-2.765982
H	-1.261053	-4.304914	-3.250833	H	-1.178080	-5.549326	-5.292583	H	-0.654402	-5.716867	-3.285627
H	-4.536657	-3.475944	1.131194	H	0.995273	-5.350259	-4.040373	H	-0.407228	-4.404692	-4.464504
H	-3.050386	-3.646373	2.105404	H	1.053139	-4.280779	-1.796291	H	-4.845438	-3.109090	-5.971381
H	-3.295021	-2.211177	1.037655	H	-2.953793	-5.222555	-0.111572	H	-5.914913	-4.274648	-5.140028
H	1.919384	-3.358497	2.275141					H	-6.068108	-2.533920	-4.780205
H	1.886316	-4.455266	0.872859					H	-5.378241	-3.154057	0.005301
H	1.788044	-2.675395	0.646962					H	-3.947766	-4.057535	0.599103
H	-0.019367	-2.388985	3.276406					H	-3.882297	-2.275768	0.396833
H	-0.061008	-1.381138	1.812362					H	2.605782	-1.609114	6.181268
H	-1.556148	-2.174272	2.403145					H	2.936588	-3.350345	6.385928
								H	4.028217	-2.360369	5.373181
								H	-2.163835	-3.349952	2.728597
								H	-1.956739	-3.016557	4.473936
								H	-1.845968	-1.680082	3.300143
								H	3.710243	-4.142755	0.985362
								H	2.373514	-5.307483	0.755631
								H	2.312023	-3.700925	-0.027618



TSG\_Monometallic



TSG\_Bimetallic

TSG_Monometallic_P <sup>t</sup> Bu <sub>3</sub>	TSG_Monometallic_PPh <sub>3</sub>	TSG_Monometallic_NHC <sup>mes</sup>
$E_{BP86} = -3972.905721$ $E_{M06} = -3971.055263$	$E_{BP86} = -4194.397303$ $E_{M06} = -4192.358607$	$E_{BP86} = -4082.352666$ $E_{M06} = -4080.206493$
C 0.267605 -1.592809 -3.352648 C -0.832284 -2.479415 -3.402599 C -0.898035 -3.646072 -4.367819 C -1.957745 -2.211240 -2.550310 O -3.043803 -2.974683 -2.843341 C -4.216931 -2.801950 -2.038724 O -2.036602 -1.361857 -1.614321 C 1.713713 -1.883080 -2.001903 C 0.769388 -1.797055 -0.925114 O 0.051570 -2.889553 -0.556950 C 0.608766 -4.028261 0.103990 O 0.330829 -0.656598 -0.539732 C 2.287199 -3.218900 -2.446541 H 2.734554 -3.116994 -3.458391 H 1.492168 -3.986278 -2.526210 H 3.086180 -3.617183 -1.780912 C 2.597953 -0.652474 -2.266486 H 0.694533 -3.814053 1.189527 H 1.595248 -4.329977 -0.300350 H -0.107421 -4.858527 -0.045647 H 0.054118 -0.564870 -3.012235 H 0.960981 -1.646088 -4.212944 H -1.751440 -3.548566 -5.074601 H -1.036658 -4.625379 -3.858051 H 0.030285 -3.707974 -4.972932 H -4.506512 -1.736179 -1.964738 H -5.012230 -3.386393 -2.538020 H -4.053694 -3.190793 -1.013022 Al -1.548793 -0.102884 -0.138844 C -0.703270 1.461526 1.039726 C -2.770517 1.259378 -1.080133 C -2.269202 -1.374472 1.288151 C -3.768807 1.938575 -0.366489 C -4.623037 2.901986 -0.935720 C -4.463550 3.229747 -2.294071 C -3.467195 2.589025 -3.051788 C -2.651613 1.627490 -2.426414 F -3.951095 1.679500 0.953068 F -5.574165 3.516602 -0.208859 F -5.257571 1.451404 -2.865167 F -3.207316 2.909402 -4.350899 C 0.036389 2.462978 0.400956 C 0.449055 3.664671 1.001514 C 0.149657 3.880239 2.357189 C -0.581004 2.906562 3.058926 C -0.983285 1.731751 2.388441 F 1.174988 4.584631 0.320986	C -0.081264 -1.668640 -3.288615 C -1.103468 -2.671502 -3.180714 C -1.088137 -3.928748 -4.027514 C -2.205920 -2.421603 -2.314525 O -3.216584 -3.331463 -2.446058 C -4.369636 -3.171458 -1.614757 O -2.350621 -1.470606 -1.477297 C 1.375418 -1.646817 -2.047764 C 0.495745 -1.645901 -0.888833 O -0.013549 -2.726383 -0.282765 C 0.435887 -0.084043 -0.371030 O -0.038673 -0.545509 -0.539693 C 2.261695 -2.833705 -2.420157 H 2.763141 -2.616680 -3.387070 H 1.687540 -3.764028 -2.579665 H 3.056484 -3.048721 -1.670898 C 2.015429 -0.269285 -2.328838 H -0.121140 -4.619275 0.420895 H 1.521192 -4.170368 -0.168196 H 0.178926 -4.528591 -1.351068 H -0.426914 -0.636390 -3.004591 H 0.536131 -1.739689 -4.206249 H -2.016856 -4.034860 -4.629867 H -1.013337 -4.870357 -3.432412 H -0.231942 -3.916282 -4.734656 H -4.791227 -2.150266 -1.689962 H -5.104470 -3.916945 -1.973555 H -4.128959 -3.368487 -0.549805 Al -1.909070 -0.030066 -0.173021 C -1.003260 1.690165 0.715025 C -3.299011 1.131406 -1.138093 C -2.464692 -1.142618 1.449195 C -4.288080 1.804392 -0.407308 C -5.265806 2.632607 -0.989890 C -5.246272 2.824097 -2.383248 C -4.263186 2.186030 -3.160604 C -3.318900 1.362419 -2.519181 F -4.332286 1.674966 0.942948 F -6.203330 3.247431 -0.245750 F -6.160852 3.615139 -2.969343 F -4.237848 2.379479 -4.493625 C -0.213970 2.523025 -0.084492 C 0.452279 3.672409 0.373543 C 0.313531 4.042570 1.720823 C -0.491896 3.263922 2.568568 C -1.120780 2.112384 2.047358 F 1.268370 4.394959 -0.439094	C 0.569627 0.723317 -3.390914 C -0.590492 0.331861 -4.137186 C -0.519377 -0.034941 -5.606028 C -1.853855 0.369446 -3.478968 O -2.912882 0.189468 -4.324123 C -4.222635 0.161768 -3.750017 O -2.089259 0.567770 -2.241898 C 1.516883 -0.570160 -2.312848 C 0.307472 -1.027379 -1.649120 O -0.544935 -1.954991 -2.102347 C -0.265919 -2.995277 -3.043532 O -0.134183 -0.341829 -0.671451 C 3.251177 -1.410971 -3.295757 H 3.096330 -0.763560 -3.765041 H 1.721440 -1.816287 -4.127739 H 2.861066 -2.259712 -2.817171 C 2.370845 0.331179 -1.407954 H -1.115999 -3.698187 -2.956968 H 0.670315 -3.532104 -2.792356 H -0.229746 -2.603683 -4.078832 H 0.367411 1.434794 -2.572113 H 1.440211 1.019805 -4.008624 H -1.200959 0.590364 -6.223265 H -0.812354 -1.090683 -5.820781 H 0.510194 0.108345 -9.996937 H -4.399014 1.027738 -3.083712 H -4.927708 0.180119 -4.602719 H -4.377829 -0.766372 -3.160011 Al -1.845042 0.483877 -0.249941 C -1.038693 0.593514 1.738336 C -2.377904 2.467750 -0.165383 C -3.312739 -0.928355 -0.069035 C -3.355203 2.883629 0.751043 C -3.771718 4.219186 0.904953 C -3.161917 5.212634 0.118163 C -2.161960 4.852791 -0.802083 C -1.797484 3.497909 -0.915347 F -3.953090 1.971786 1.559088 F -4.724410 4.562640 1.791188 F -3.529681 6.498875 0.247587 F -1.566375 5.805361 -1.546850 C 0.105939 1.373404 1.937678 C 0.723551 1.594643 3.180940 C 0.169009 0.999307 4.326870 C -0.990473 0.215412 4.194471 C -1.557095 0.032027 2.914243 F 1.848255 2.348700 3.292164



F	0.560328	5.003854	2.973011	F	0.960908	5.127918	2.194377	F	0.737184	1.182825	5.532310
F	-0.872733	3.107212	4.358041	F	-0.628310	3.616904	3.859809	F	-1.530010	-0.353960	5.289323
F	-1.692816	0.858404	3.143176	F	-1.861284	1.410166	2.936176	F	-2.672118	-0.736447	2.887279
C	-1.426873	-2.011106	2.206558	C	-1.535088	-1.570495	2.403424	C	-3.049966	-2.249266	0.313945
C	-1.862816	-2.922122	3.182906	C	-1.843303	-2.397789	3.495935	C	-4.040027	-3.238121	0.446796
C	-3.235853	-3.211717	3.272625	C	-3.173027	-2.816607	3.675053	C	-5.379067	-2.907021	0.177979
C	-4.132468	-2.586366	2.388434	C	-4.155977	-2.394526	2.762060	C	-5.699468	-1.592567	-0.202199
C	-3.626442	-1.694734	1.421783	C	-3.776963	-1.578487	1.677269	C	-4.662300	-0.646731	-0.324508
F	-0.989970	-3.527887	4.015830	F	-0.885116	-2.801544	4.360886	F	-3.731206	-4.503389	0.817822
F	-3.685654	-4.079118	4.194633	F	-3.501174	-3.608132	4.709141	F	-6.342207	-3.836072	0.292930
F	-5.446876	-2.862122	2.467368	F	-5.430594	-2.790508	2.928314	F	-6.979367	-1.267703	-0.460277
F	-4.544154	-1.141143	0.589062	F	-4.772023	-1.224970	0.826873	F	-5.042658	0.597067	-0.710061
H	2.008158	0.050335	-2.897897	H	1.235889	0.395777	-2.759244	H	1.807168	1.263781	-1.211055
H	3.443837	-0.967355	-2.909644	H	2.785523	-0.385219	-3.120817	H	3.289781	0.633295	-1.951571
P	4.632853	0.124950	-0.104887	P	4.104647	0.127748	-0.274454	C	3.941727	-1.024345	0.229698
C	6.105479	-0.435625	-1.227297	C	5.511928	0.021682	-1.433270	F	-1.775469	-2.642170	0.600660
C	4.340563	-1.080511	1.378013	C	3.933198	-1.418848	0.672750	F	0.705117	2.001413	0.873720
C	4.905987	1.947280	0.525192	C	4.447570	1.452167	0.936996	F	-0.805666	3.229712	-1.810030
F	-0.077748	-1.771251	2.191253	F	-0.225857	-1.182019	2.318501	N	5.229310	-0.563748	0.227592
F	0.403802	2.310027	-0.913423	F	-0.036477	2.233360	-1.413509	C	6.097572	-1.598649	0.561959
F	-1.699318	1.056258	-3.216387	F	-2.384604	0.789069	-3.327561	C	5.329492	-2.713806	0.776663
C	3.082202	0.277899	-1.115514	C	5.596882	-1.048723	-2.356116	N	4.001444	-2.348990	0.565441
H	3.213568	1.288732	-1.554833	C	6.643040	-1.083147	-3.292099	C	2.880902	-3.263685	0.688523
H	2.247576	0.394789	-0.389578	C	7.603667	-0.056157	-3.318347	H	5.600824	-3.730023	1.076513
C	5.864172	1.993265	1.736941	C	7.520267	1.008560	-2.404767	H	7.177677	-1.438959	0.632355
C	5.479583	2.845175	-0.596960	C	6.479355	1.052246	-1.462246	C	5.638713	0.802883	-0.035379
C	3.541508	2.561048	0.922107	H	4.850508	-1.856740	-2.345172	C	2.759848	-4.306094	-0.266136
C	7.470850	-0.112960	-0.576561	H	6.705418	-1.918550	-4.006625	C	1.657727	-5.173867	-0.143572
C	6.032633	-1.958190	-1.491267	H	8.421315	-0.086658	-4.055411	C	0.699113	-5.034700	0.880323
C	6.018607	0.282441	-2.598379	H	8.270685	1.814061	-2.422413	C	0.886787	-4.008956	1.827068
C	5.643459	-1.398545	2.145702	H	6.420919	1.888437	-0.748632	C	1.970767	-3.113318	1.766812
C	3.298119	-0.463300	2.344117	C	5.369160	1.188884	1.978683	C	3.780623	-4.537600	-1.360253
C	3.740782	-2.399473	0.846959	C	5.640583	2.177355	2.936082	H	1.542455	-5.985886	-0.880730
H	5.487126	3.887113	-0.213024	C	4.984421	3.421208	2.872932	C	-0.504705	-5.939536	0.964640
H	6.520432	2.595848	-0.878277	C	4.064019	3.681706	1.844503	H	0.153528	-3.887140	2.640229
H	4.848029	2.851064	-1.507815	C	3.798396	2.704977	0.868490	C	2.108889	-2.047143	2.828604
H	6.029300	3.059507	1.999883	H	5.862251	0.206478	2.051569	C	5.566810	1.754924	1.010346
H	5.438539	1.506686	2.634845	H	6.355442	1.968180	3.747021	C	5.965407	3.073472	0.708613
H	6.856980	1.550389	1.528607	H	5.183727	4.187331	3.638516	C	6.424963	3.448759	-0.568148
H	3.738106	3.550458	1.385633	H	3.520940	4.637609	1.803104	C	6.508945	2.454397	-1.566035
H	2.891183	2.752645	0.050039	C	3.069266	2.940884	0.080460	C	6.128065	1.121652	-1.327871
H	2.968734	1.967084	1.653925	C	4.964197	-2.383992	0.729509	C	5.081586	1.410559	2.399852
H	8.269778	-0.520711	-1.232162	C	4.816270	-3.506870	1.563314	H	5.913103	3.831447	1.507452
H	7.655004	0.973909	-0.481940	C	3.654441	-3.663546	2.340735	C	6.795487	4.881842	-0.870235
H	7.596976	-0.576802	0.419854	C	2.630530	-2.699638	2.288505	H	6.884030	2.724411	-2.566923
H	6.882689	-0.054876	-3.209784	C	2.765357	-1.576396	1.456258	C	6.263859	0.073427	-2.409553
H	5.102716	0.022258	-3.161499	H	5.880008	-2.262332	0.130775	H	-1.434853	-5.550766	0.822484
H	6.080752	1.381105	-2.524973	H	5.618138	-4.260384	1.606686	H	-0.475420	-6.739747	0.199374
H	6.797463	-2.206299	-2.257917	H	3.547309	-4.542153	2.996358	H	-0.578292	-6.418683	1.963439
H	6.270336	-2.559428	-0.593122	H	1.714017	-2.804052	2.888698	H	3.317496	-5.050020	-2.226356
H	5.052049	-2.284270	-1.888165	H	1.952363	-0.834894	1.437492	H	4.242785	-3.600086	-1.728108
H	5.378247	-2.048656	3.006527	C	2.569940	0.579527	-1.162322	H	4.609849	-5.191200	-1.009860
H	6.371747	-1.964939	1.532585	H	2.786409	1.600824	-1.543386	H	7.573101	4.948118	-1.657298
H	6.146088	-0.503896	2.556435	H	1.781773	0.693537	-0.386259	H	5.908850	5.444199	-1.237046
H	3.451571	-3.017100	1.722832					H	7.164703	5.408894	0.032025
H	2.822935	-2.226692	0.252424					H	5.651055	1.979959	3.161181
H	4.449968	-2.992881	0.244061					H	4.012553	1.681980	2.540715
H	3.064625	-1.228324	3.113924					H	5.188983	0.333164	2.634855
H	3.670809	0.430596	2.878719					H	7.105756	-0.622796	-2.203022
H	2.336421	-0.220542	1.848820					H	5.350254	-0.548317	-2.510349
								H	6.461417	0.545232	-3.391276
								H	3.130534	-1.623521	2.889196
								H	1.402353	-1.207466	2.648446
								H	1.855610	-2.461214	3.824638
								C	2.725267	-0.194222	0.020971
								H	2.843531	0.698889	0.668748
								H	1.845120	-0.730333	0.420323





C	3.115533	3.807448	-0.919189	C	1.249909	7.998346	-0.396975	C	-0.492571	0.843450	4.811337
C	1.806182	5.397517	-2.306467	C	-0.138782	8.200500	-0.286968	C	-1.466577	1.526156	4.055493
H	-3.274867	5.258530	-0.218735	C	-1.002418	7.099744	-0.164520	C	-1.125426	2.489624	3.087265
H	-2.597906	3.641951	0.084420	C	-0.486915	5.791575	-0.137980	C	2.743522	2.380394	3.431137
H	-2.336083	4.970167	1.263976	H	2.861087	6.545703	-0.485947	H	1.640979	0.604791	5.143709
H	-1.870741	7.235617	-0.586744	H	1.928862	8.858743	-0.502346	C	-0.893237	-0.165013	5.862786
H	-0.644216	6.927371	0.671265	H	-0.548923	9.222346	-0.305711	H	-2.531760	1.295925	4.212614
H	-0.152810	7.128481	-1.045149	H	-2.090644	7.250305	-0.096129	C	-2.213801	3.214880	2.327726
H	-2.355583	5.626052	-2.367656	H	-1.187777	4.948189	-0.062927	C	0.935644	5.564549	-2.125082
H	-0.680990	5.219874	-2.812948	C	4.127983	3.641101	-1.582241	C	1.486497	5.985155	-3.349520
H	-1.835736	3.929769	-2.329105	C	4.927122	3.666004	-2.738985	C	2.864086	6.254713	-3.501423
H	0.363229	4.989302	3.612949	C	4.345135	3.904548	-3.994265	C	3.704349	6.086055	-2.383831
H	0.948780	5.999489	2.264374	C	2.956921	4.121677	-4.100456	C	3.214565	5.664611	-1.129918
H	-0.793306	5.567317	2.389437	C	2.150067	4.094624	-2.953109	C	-0.543246	5.292770	-1.986432
H	4.040026	4.259933	-1.334759	H	4.600745	3.462077	-0.607094	H	0.812463	6.109448	-4.213066
H	3.377048	3.378219	0.063614	H	6.008180	3.488416	-2.641712	C	3.411169	6.738820	-4.824426
H	2.841424	2.975997	-1.596211	H	4.975016	3.929158	-4.897405	H	4.782961	6.291035	-2.829599
H	3.428265	6.517034	-0.493649	H	2.500315	4.322872	-5.082119	C	4.157302	5.465858	0.033725
H	1.785410	6.910859	0.083342	H	1.070303	4.295706	-3.042892	H	3.277968	2.337782	4.400899
H	2.834099	5.790047	1.017463	H	1.998482	5.639817	2.160200	H	3.209084	1.610140	2.779502
H	2.793271	5.715749	-2.703289	C	0.267406	2.704219	-0.253077	H	2.937700	3.374855	2.982995
H	1.435090	4.599201	-2.979969	H	-0.323803	3.012309	0.637031	H	-1.979323	-0.378994	5.828948
H	1.129591	6.269305	-2.378495	H	-0.359866	2.964147	-1.131240	H	-0.341358	-1.117768	5.733674
H	1.873443	3.155028	3.273306					H	-0.655564	0.210893	6.881462
H	2.167622	2.384846	1.705098					H	-1.971966	3.354433	1.255824
H	2.714352	4.077798	2.003029					H	-3.159743	2.645471	2.383762
H	-0.437269	2.663117	3.284702					H	-2.413081	4.222284	2.754077
H	-1.583914	3.099431	1.994311					H	3.692147	5.723811	1.006607
H	-0.350099	1.828374	1.715852					H	4.503707	4.411807	0.097614
								H	5.064894	6.088959	-0.084322
								H	4.512500	6.632905	-4.878188
								H	2.966359	6.184869	-5.676335
								H	3.172276	7.813610	-4.979954
								H	-1.061393	5.412778	-2.956524
								H	-0.753871	4.265383	-1.623414
								H	-1.029092	5.984257	-1.266320



		H	6.098439	1.295535	-3.536834
		H	3.286483	-3.730303	1.822478
		H	2.416912	-2.175304	1.969900
		H	1.780551	-3.622697	2.789683
		C	2.309134	-0.225340	-0.200650
		H	2.640475	0.314946	0.710203
		H	1.369741	-0.755439	0.050417

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