

Supplementary Information

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

Yuetao Zhang,[†] Garret M. Miyake,[†] Mallory G. John,[†] Laura Falivene,[‡] Lucia Caporaso,[‡] Luigi

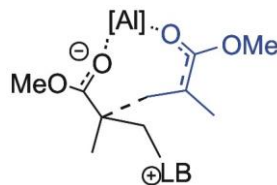
Cavallo,^{*,§} and Eugene Y.-X. Chen^{*,†}

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

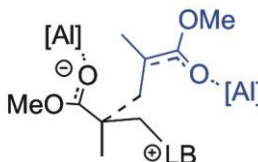
Al(C ₆ F ₅) ₃	MMA	Al(C ₆ F ₅) ₃ -MMA
E _{BP86} =-2426.735258 E _{M06} =-2425.720189	E _{BP86} =-345.906991 E _{M06} =-345.678099	E _{BP86} =-2772.683230 E _{M06} =-2771.459124
Al -0.002935 -0.000305 0.000580 C 0.871598 1.761106 0.000141 C 2.139463 4.300204 -0.000262 F 2.736241 5.493717 -0.001060 C 0.604313 2.713995 -0.994040 C 1.218118 3.978125 -1.017687 F -0.268063 2.410393 -1.982238 F 0.951309 4.867119 -1.980674 C -1.965518 -0.124670 0.001279 C -4.797829 -0.303386 0.000431 C -2.655237 -0.835148 -0.992492 C -2.739532 0.493425 0.994745 C -4.142952 0.420264 1.017862 C -4.056553 -0.939358 -1.016380 F -1.954258 -1.437701 -1.980134 F -2.120623 1.179613 1.982586 F -4.858535 1.014112 1.979316 F -4.691249 -1.617909 -1.978605 F -6.129609 -0.387091 -0.000147 C 1.793797 2.120496 0.994385 C 2.434916 3.370979 1.018147 F 2.075144 1.240649 1.982706 F 3.306727 3.691861 1.980506 C 1.087171 -1.636981 0.000894 C 2.664031 -3.996358 -0.001779 C 2.042896 -1.879054 -0.997066 C 0.945773 -2.614306 0.997325 C 1.714018 -3.791127 1.019683 C 2.836520 -3.038721 -1.022060 F 2.206981 -0.971772 -1.987229 F 0.045773 -2.421301 1.988677 F 1.564946 -4.705640 1.984402 F 3.737304 -3.249548 -1.988098 F 3.405491 -5.105718 -0.002927	C -0.979046 -0.679498 0.000000 C 0.000000 0.466041 0.000000 C -2.288764 -0.341239 0.000000 C -0.489119 -2.114546 0.000000 H -3.080439 -1.108016 0.000000 H -2.582754 0.719953 0.000000 H 0.613722 -2.169228 0.000000 H -0.860140 -2.660142 0.892972 H -0.860140 -2.660142 -0.892972 O 1.293676 0.034126 0.000000 O -0.297382 1.650312 0.000000 C 2.284827 1.071323 0.000000 H 3.264546 0.559327 0.000000 H 2.183732 1.715130 -0.898054 H 2.183732 1.715130 0.898054	Al -0.013571 0.032652 0.126754 C -1.578685 -1.173346 -0.235239 C -2.857963 -0.787838 0.196569 C -4.021804 -1.533682 -0.058173 C -3.906566 -2.742265 -0.771723 C -2.644329 -3.181551 -1.212663 C -1.514777 -2.391741 -0.928009 C -0.344487 1.985817 -0.186528 C 0.414842 2.968502 0.463533 C 0.233677 4.349833 0.277652 C -0.757462 4.781627 -0.624000 C -1.540954 3.835822 -1.311544 C -1.314451 2.465472 -1.081508 C 1.791347 -0.524423 -0.546457 C 1.930906 -0.632175 -1.938099 C 3.136911 -0.963820 -2.578269 C 4.276777 -1.192514 -1.783226 C 4.191118 -1.086899 -0.382344 C 2.955208 -0.751016 0.201304 F 2.936304 -0.645184 1.556239 F 5.281498 -1.300563 0.370125 F 5.442103 -1.507678 -2.359467 F 3.223655 -1.057072 -3.912009 F 0.849813 -0.397856 -2.722934 F -2.536254 -4.340938 -1.877375 F -0.316592 -2.874030 -1.340051 F -4.995769 -3.476926 -1.022280 F -5.224310 -1.125179 0.371961 F -3.007455 0.360011 0.904832 F -2.080916 1.597787 -1.778305 F -2.480178 4.251223 -2.172493 F -0.953946 6.089299 -0.826362 F 0.981882 5.250022 0.934050 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

P^tBu₃	PPh₃	PMes₃	NHC^{mes}	PMe₃
E_{BP86}==815.0478372 E_{M06}==814.6374144	E_{BP86}==1036.540481 E_{M06}==1035.937736	E_{BP86}==1390.455731 E_{M06}==1389.589633	E_{BP86}==924.4429528 E_{M06}==923.7365278	E_{BP86}==461.1748458 E_{M06}==461.0187089
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 0.122464 -0.795912 H -2.405120 -1.035163 -1.975719 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 -0.994755 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 C 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 -3.354765 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 0.160406 C 2.985290 1.226933 -0.381524 C 4.333831 1.216228 -0.784120 C 5.144688 0.068449 -0.665424 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 1.092394 -0.139686 C -3.222892 1.143571 0.278148 C -2.125311 -2.463799 -0.529877 H -4.752728 -2.149419 -1.207990 H -5.183322 2.005158 -0.057413 C -2.629097 2.428505 0.810042 C 6.587971 0.093341 -1.115962 C -6.592028 -0.118386 -1.102806 H 2.728849 3.307209 -0.946985 H 1.278189 2.266225 -1.213948 H 1.702186 2.787663 0.433426 C 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

[Al]-MMA-P'Bu ₃			[Al]-MMA-PPh ₃			[Al]-MMA-PMes ₃			[Al]-MMA-NHC ^{mes}			[Al]-MMA-PMe ₃							
E _{BP86} =−3587.731731			E _{BP86} =−3809.221778			E _{BP86} =4163.1080134			E _{BP86} =3697.168215			E _{BP86} =−3233.869853							
E _{M06} =−3586.121534			E _{M06} =−3807.417607			E _{M06} =−4161.049428			E _{M06} =−3695.261185			E _{M06} =−3232.501166							
Al	1.414170	-0.026403	-0.114471	Al	1.659835	0.104786	0.101363	Al	-2.277123	0.352326	-0.229062	Al	1.737280	0.093504	-0.037660	Al	-0.468827	0.026570	-0.116939
C	0.701899	-1.414347	1.191361	C	1.380137	1.841529	-0.910479	C	-2.533652	2.356020	-0.389737	C	1.264299	-1.082300	-1.627486	C	-0.259630	1.778429	0.877452
C	0.865301	-2.774930	0.892954	C	1.952187	3.028454	-0.420591	C	-3.533114	2.926262	-1.138252	C	1.726499	-0.798586	-2.921350	C	-1.052603	2.908371	0.627985
C	0.375064	-3.820091	1.666259	C	1.825994	4.273834	-1.070938	C	-3.674101	4.312623	-1.219666	C	1.422393	-1.580624	-4.051129	C	-0.900599	4.132693	1.304891
C	-0.346662	-3.494903	1.860351	C	1.067421	4.350741	-2.253926	C	-2.755774	5.206399	-0.533473	C	0.588200	-2.702104	-3.892930	C	0.116477	4.252192	2.269758
C	-0.553988	-2.145002	3.196922	C	0.455697	3.193157	-2.768708	C	-1.722409	4.617019	0.218277	C	0.085835	-3.021389	-2.619218	C	0.953418	3.154904	2.542759
C	-0.021665	-1.147263	2.359396	C	0.623050	1.978070	-2.080272	C	-1.636773	3.215114	0.260948	C	0.428598	-2.203967	-1.526833	C	0.750766	1.957818	1.832796
C	3.324095	-0.353568	-0.692176	C	3.554832	-0.167909	0.753947	C	-3.779902	-0.830414	-0.903622	C	3.597538	0.892078	-0.067013	C	-2.319969	-0.404343	-0.804353
C	3.840593	0.326701	-1.804387	C	3.833142	-1.063910	1.795946	C	-3.645412	-1.998518	-1.664761	C	3.890346	2.040430	0.682202	C	-2.511215	-1.232807	-1.919446
C	5.166093	0.200708	-2.255938	C	5.127597	-1.336083	2.273178	C	-4.718527	-2.846918	-1.992092	C	5.164465	6.232534	0.745673	C	-3.774055	-1.616198	-2.405276
C	6.038626	-0.646991	-1.548253	C	6.218149	-0.685994	1.666594	C	-6.007495	-2.519392	-1.534797	C	6.218843	2.038018	0.028814	C	-4.921560	-1.157358	-1.732556
C	5.574381	-1.344889	-0.418312	C	5.996077	0.214909	0.690908	C	-6.198397	-1.360442	-0.759296	C	5.981917	0.877391	-0.730156	C	-4.786308	-0.332170	-0.601243
C	4.235155	-1.178891	-0.014894	C	4.676426	0.448189	1.765058	C	-5.082567	-0.586260	-0.457680	C	4.684551	3.30617	-0.755483	C	-3.495328	0.018829	-0.162031
C	1.358584	1.873253	0.580040	C	1.158112	-1.562737	-0.934109	C	-2.063165	-0.281576	1.689732	C	1.614338	-0.494048	1.708971	C	0.083539	-1.569466	1.025666
C	2.047174	2.130044	1.775726	C	1.731152	-1.738126	-2.203142	C	-2.392831	0.458184	2.836070	C	2.611731	-1.906440	1.955681	C	-0.714545	-1.912729	2.121995
C	2.152740	3.403130	2.363738	C	1.520092	-2.869225	3.3011697	C	-2.342107	-0.072774	4.140848	C	2.678855	-2.691650	3.122062	C	-0.441071	-2.992079	2.991696
C	1.539313	4.494529	1.720464	C	0.697105	-3.900164	-2.521777	C	-1.951130	-1.412765	4.139435	C	1.684076	-0.591943	4.103811	C	0.700537	-3.781014	2.755245
C	0.841964	-2.920568	0.515351	C	0.115907	-3.783266	-1.247518	C	-1.621328	-2.191397	3.200662	C	0.659054	-1.590815	3.903581	C	1.530991	-3.470675	1.661917
C	0.778930	2.994386	-0.025144	C	0.353156	-2.625025	-0.491534	C	-1.693981	-1.613339	9.24318	C	0.653829	-0.561177	2.717088	C	1.194546	-2.392797	0.839114
F	0.094274	2.873032	-1.194726	F	-0.243034	2.575328	0.728914	F	-1.375224	2.410480	0.871855	F	-0.392482	0.036282	5.81385	F	2.061945	-2.156340	-0.006040
F	0.245878	5.331845	-0.095546	F	-0.665853	-4.774915	-0.779204	F	-1.241597	-3.749616	3.367374	F	-0.309902	-1.446786	4.829310	F	2.640125	-2.412429	1.429052
F	1.615197	5.721118	2.255354	F	0.462406	-0.989908	-3.269057	F	-1.894757	-1.939164	5.551543	F	1.710521	-3.272291	5.209897	F	0.993102	-0.848198	3.562770
F	8.202611	3.595368	3.511669	F	2.081698	-2.982695	-4.225832	F	-2.663611	0.672617	5.211019	F	3.656305	-3.592418	3.305056	F	-1.237462	-3.273479	4.032418
F	2.657335	1.105286	2.405663	F	2.546620	-0.776305	-2.700628	F	-2.796185	1.743853	2.731984	F	3.576712	-1.18810	1.029742	F	-1.813775	-1.177319	2.014927
F	-1.272520	-1.828487	4.290885	F	-0.286559	3.266860	-3.887511	F	-0.837491	5.396340	0.863720	F	-0.731497	-4.085055	-2.473977	F	1.936813	3.273549	3.451502
F	-0.280151	0.138038	2.733353	F	-0.026484	0.898748	-2.603789	F	-0.608176	6.956124	0.988925	F	-0.115878	-2.548528	-0.328744	F	1.612317	0.939872	2.114102
F	-0.843209	-4.666827	3.638783	F	0.920646	5.524486	-2.883497	F	-2.860033	6.545092	-0.600150	F	0.626870	-3.640491	-4.951694	F	0.291827	5.409012	2.922420
F	0.560059	-5.107870	1.366137	F	2.396442	5.381822	-0.573034	F	-4.649856	5.954951	-1.949246	F	1.893257	-1.268017	-0.5268753	F	-1.688380	5.184930	1.034597
F	1.518391	-3.137033	-0.240150	F	2.669591	3.009184	0.722797	F	-4.418822	2.527646	-1.857701	F	2.507033	0.288569	-3.138496	F	-2.023402	2.863632	-0.318981
F	3.852571	-1.859003	1.089748	F	4.526528	1.307813	-0.857185	F	-5.303067	0.522165	0.330320	F	4.523172	-0.796649	-1.483503	F	-3.425777	0.795266	0.941243
F	6.412399	-2.147639	0.256591	F	7.039791	0.827908	0.028561	F	-7.425948	-1.053045	-0.312103	F	6.993076	0.308948	-1.407029	F	-5.882872	0.097745	0.042071
F	7.730074	-0.788923	-1.950331	F	7.465119	-0.925145	0.295006	F	-7.048233	-3.308969	-1.831952	F	7.446312	2.575777	0.069807	F	-6.139651	-1.506786	-2.168075
F	5.609622	0.869037	-3.333714	F	5.333845	-2.198660	3.281672	F	-4.527171	-3.963699	-2.717680	F	5.390444	3.739610	1.474422	F	-3.901120	-2.047629	-3.484143
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C	-1.701256	-1.619706	-1.496399	C	-1.385858	1.728948	1.744825	C	-1.277872	1.245699	-1.804339	C	-1.603361	1.379004	-1.263818	C	2.669916	1.512910	-1.054847
C	-0.468575	-1.201395	-1.981551	C	-0.180300	1.171099	2.162021	C	-0.004561	1.753741	-0.203079	C	-0.323611	1.857901	-1.058169	C	1.374036	1.177478	-2.096844
C	-2.336277	-0.824749	-0.403177	C	-1.961308	1.313855	0.445967	C	1.879486	1.018210	-0.476557	C	-1.211250	0.309089	-0.336836	C	3.450270	0.704339	-0.837744
C	-2.311600	-2.095925	-1.989259	C	-2.111014	2.753751	2.578730	C	1.988967	2.079494	-2.844720	C	-2.409307	1.747139	-2.482032	C	3.361428	2.669387	-0.562096
H	-1.532143	-3.367955	-2.417678	H	-2.436426	3.624890	1.964914	H	2.988234	1.673226	-3.123436	H	-2.649025	0.846817	-3.098764	H	2.631049	3.480314	-2.755435
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O	0.012073	-1.877517	-3.065537	O	0.298989	1.576004	3.396652	O	-0.503929	0.974581	-3.295194	O	0.115035	2.855302	-1.877803	O	0.742925	1.899538	-3.067011
O	0.243841	-1.901256	-1.522636	O	0.500755	0.261381	1.508341	O	-0.736027	0.078672	-1.183996	O	0.495713	1.442098	-0.097656	O	0.715907	0.203268	-1.506662
C	1.378259	-1.668890	-1.454681	C	1.644326	1.229492	3.711972	C	-1.823828	0.533536	-3.622479	C	1.470168	3.296097	-1.765744	C	-0.643941	1.647449	-3.319789
H	1.491113	-2.203565	-4.402323	H	1.764437	1.526288	4.777852	H	-1.950073	0.750768	-4.699896	H	1.536317	4.227075	-2.370674	H	-0.886323	2.208468	-4.242052
H	1.624378	-0.612458	-3.558781	H	1.827744	0.142890	3.608437	H	-1.841319	-0.523419	-3.441537	H	1.743628	3.512590	-0.713653	H	-0.834412	0.566330	-3.472391
H	2.068900	-2.143557	-2.708795	H	2.373179	1.787497	3.094966	H	-2.602897	1.087999	-3.058509	H	2.176555	2.544461	-2.176386	H	-1.282466	2.019722	-2.491666
P	-3.943793	0.183472	0.366995	P	-3.466113	0.096290	0.484541	P	3.306649	-0.316455	-0.180122	C	-3.458248	0.503923	0.296724	P	4.494109	-0.618238	-1.629572
P	-2.579589	-1.433253	0.496804	H	-2.357578	2.165579	-0.138228	P	2.318524	1.922044	-0.010174	H	-2.160956	-0.693900	-0.814023	H	1.610585	1.304017	-0.223171
H	-1.624100	-0.445736	-0.071332	H	-1.230312	0.772266	-0.198288	H	1.112627	0.614633	0.201972	H	-1.390178	0.190779	0.502732	H	2.775972	0.160162	-0.146034
C	-3.878872	1.149986	0.824848	C	-3.629524	-0.663006	2.123601	C	2.503378	-1.945561	-0.499487	N	-4.086227	1.645639	0.710809	C	3.520695	-1.528177	-2.865573
C	-5.485154	-0.986545	-0.439125	C	-3.243379	-1.208947	0.766946	C	3.814451	-0.017496	1.591981	C	-5.289560	1.306889	1.332534	H	1.613005	-2.622710	-3.390352
C	-5.801942	-1.720200	-1.762853	C	-4.864810	-0.691174	2.809776	C	2.322511	-9.257173	0.531023	C	-5.408782	-0.056516	1.287365	H	2.684387	-2.041257	-2.354643
C	-5.168221	-2.074275	-0.617927	C	-4.940205	-1.286743	4.079049	C											



TS1_Monometallic



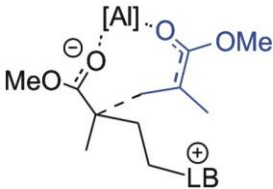
TS1_Bimetallic

TS1_Monometallic_P ^t Bu ₃	TS1_Monometallic_PPh ₃	TS1_Monometallic_NHC ^{mes}
E _{BP86} =-3933.587583 E _{M06} =-3931.766374	E _{BP86} =-4155.079299 E _{M06} =-4153.066668	E _{BP86} =-4043.032628 E _{M06} =-4040.919687
C -1.135049 -1.004329 2.981809 C -0.116612 -1.858107 3.465209 C -0.336589 -2.818661 4.617414 C -1.192003 -1.760319 2.878993 O 2.136721 -2.461439 3.557821 C 3.470972 -2.462372 3.032095 O 1.530795 -1.108591 1.849062 C -2.211371 -1.596746 1.403654 C -1.033477 -1.648265 0.565153 O -0.314829 -2.793136 0.499465 C -0.818358 -3.983755 -0.120086 O -0.469431 -0.578375 0.164830 C -8.231398 -2.873944 1.944266 H -3.438181 -2.655246 2.842882 H -2.020910 -3.560539 2.278263 H -3.468258 -3.429815 1.229764 C -3.066280 -0.346970 1.242779 H -0.365643 -0.064775 -1.129498 H -1.921441 -3.976263 -0.221743 H -0.510889 -4.849939 0.497732 H -0.804434 -0.057304 2.521781 H -2.014410 -0.902793 3.646570 H 0.336456 -2.590897 5.472942 H -0.135593 -3.879613 4.348394 H -1.380515 -2.755753 4.989183 H 3.821809 -1.436741 2.810398 H 4.100897 -2.929757 3.811744 H 3.525222 -3.059506 2.098623 Al 1.465116 -0.071504 0.140221 C 0.931038 1.283570 -1.395861 C 2.485138 1.406670 1.145770 C 2.481908 -1.530339 -0.857559 C 3.625597 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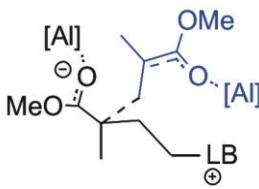
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H	-3.948290	3.725646	0.853033
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H	-3.828980	-2.420037	-1.709130
H	1.399199	-0.334730	1.342217
H	4.756214	-3.826672	-1.045274
H	4.945527	-5.305095	-0.063570
H	7.635210	4.904957	-1.627431
H	5.910217	5.370741	-1.690188
H	6.823630	5.577643	-0.171006
H	4.272100	2.711373	2.813633
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

TS1_Bimetallic_P ^t Bu ₃	TS1_Bimetallic_PPh ₃	TS1_Bimetallic_NHC ^{mes}
E _{BP86} == -6360.391808 E _{M06} == -6357.575911	E _{BP86} == -6581.88187 E _{M06} == -6578.8776	E _{BP86} == -6469.830265 E _{M06} == -6466.723066
C -0.064764 0.520669 -1.972695 C 1.292422 0.168447 -1.684003 C 2.248002 -0.307274 -2.760131 C 1.789669 0.344485 -0.366049 O 0.903543 0.719847 0.589160 C 1.427081 1.130756 1.869361 O 3.009687 0.165717 -0.013425 C -1.324403 -1.049929 -1.986954 C -2.582268 -0.370004 -1.701164 O -3.393634 0.206109 -2.600023 C -3.127863 0.630040 -3.947941 O -3.003920 -0.220801 -0.499229 C -1.126602 -1.645127 -3.376959 H -0.130910 -2.122051 -3.443057 H -1.147278 -0.887049 -4.180093 H -1.890831 -2.412422 -3.627635 C -0.764626 -1.833080 -0.730345 H -3.950108 1.331149 -4.180452 H -3.163852 -0.221661 -4.655101 H -2.163260 1.165521 -4.021176 H -0.560762 1.153359 -1.222643 H -0.255412 0.839113 -3.011495 H 3.176261 0.301625 -2.793463 H 1.776739 -0.236226 -3.760931 H 2.579181 -1.357229 -2.611262 H 2.032175 2.054184 1.764727 H 0.538821 1.317725 2.497943 H 2.056209 0.332657 2.309161 Al 4.826436 0.454244 -0.039299 C 5.444602 0.407931 1.884760 C 5.691760 -1.093910 -1.013243 C 4.966437 2.258582 -0.924664 Al -4.490363 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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
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H -3.575153 -2.581719 -1.507709	C -2.322336 -3.966618 -2.464920	C -2.062967 -4.069539 -3.102586
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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 ^t Bu ₃	TSG_Monometallic_PPh ₃	TSG_Monometallic_NHC ^{mes}
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 -0.539372 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 -1.374742 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 4.151404 -2.865167 F -3.307316 2.909402 -4.350899 C 0.036389 2.462978 0.400956 C 0.449055 3.664671 1.001514 C 1.149657 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 -4.084043 -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 -3.094591 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 3.235177 -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 1.018905 -4.008624 H -1.200959 0.590364 -6.223265 H -0.812354 -1.090683 -5.820781 H 0.510194 0.108345 -5.996937 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

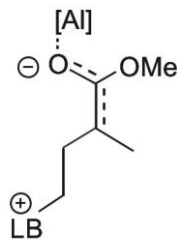
F	0.560328	5.003854	2.973011
F	-0.872733	3.107212	4.358041
F	-1.692816	0.858404	3.143176
C	-1.426873	-2.011106	2.206558
C	-1.862816	-2.922122	3.182906
C	-3.235853	-3.211717	3.272625
C	-4.132468	-2.586366	2.388434
C	-3.626442	-1.694734	1.421783
F	-0.989970	-3.527887	4.015830
F	-3.685654	-4.079118	4.194633
F	-5.446876	-2.862122	2.467368
F	-4.544154	-1.141143	0.589062
H	2.008158	0.050335	-2.897897
H	3.443837	-0.967355	-2.909644
P	4.632853	0.124950	-0.104887
C	6.105479	-0.435625	-1.227297
C	4.340563	-1.080511	1.378013
C	4.905987	1.947280	0.525192
F	-0.077748	-1.771251	2.191253
F	0.403802	2.310027	-0.913423
F	-1.699318	1.056258	-3.216387
C	3.082202	0.277899	-1.115514
H	3.213568	1.288732	-1.554833
H	2.247576	0.394789	-0.389578
C	5.864172	1.993265	1.736941
C	5.479583	2.845175	-0.596960
C	3.541508	2.561048	0.922107
C	7.470850	-0.112960	-0.576561
C	6.032633	-1.958190	-1.491267
C	6.018607	0.282441	-2.598379
C	5.643459	-1.398545	2.145702
C	3.298119	-0.463300	2.344117
C	3.740782	-2.399473	0.846959
H	5.487126	3.887113	-0.213024
H	6.520432	2.595848	-0.878277
H	4.848029	2.851064	-1.507815
H	6.029300	3.059507	1.999883
H	5.438539	1.506686	2.634845
H	6.856980	1.550389	1.528607
H	3.738106	3.550458	1.385633
H	2.891183	2.752645	0.050039
H	2.968734	1.967084	1.653925
H	8.269778	-0.520711	-1.232162
H	7.655004	0.973909	-0.481940
H	7.596976	-0.576802	0.419854
H	6.882589	-0.054876	-3.209784
H	5.102716	0.022258	-3.161499
H	6.080752	1.381105	-2.524973
H	6.797463	-2.206299	-2.257917
H	6.270336	-2.559428	-0.593122
H	5.052049	-2.284270	-1.888165
H	5.378247	-2.048656	3.006527
H	6.371747	-1.964939	1.532585
H	6.146088	-0.503896	2.556435
H	3.451571	-3.017100	1.722832
H	2.822935	-2.226692	0.252424
H	4.449968	-2.992881	0.244061
H	3.064625	-1.228324	3.113924
H	3.670809	0.430596	2.878719
H	2.336421	-0.220542	1.848820

F	0.960908	5.127918	2.194377
F	-0.628310	3.616904	3.859809
F	-1.861284	1.410166	2.936176
C	-1.535088	-1.570495	2.403424
C	-1.843303	-2.397789	3.495935
C	-3.173027	-2.816607	3.675053
C	-4.155977	-2.394526	2.762060
C	-3.776963	-1.578487	1.677269
F	-0.885116	-2.801544	4.360886
F	-3.501174	-3.608132	4.709141
F	-5.430594	-2.790508	2.928314
F	-4.772023	-1.224970	0.826873
H	1.235889	0.395777	-2.759244
H	2.785523	-0.385219	-3.120817
P	4.104647	0.127748	-0.274454
C	5.511928	0.021682	-1.433270
C	3.933198	-1.418848	0.672750
C	4.447570	1.452167	0.936996
F	-0.225857	-1.182019	2.318501
F	-0.036477	2.233360	-1.413509
F	-2.384604	0.789069	-3.327561
C	5.596882	-1.048723	-2.356116
C	6.643040	-1.083147	-3.292099
C	7.603667	-0.056157	-3.318347
C	7.520267	1.008560	-2.404767
C	6.479355	1.052246	-1.462246
H	4.850508	-1.856740	-2.345172
H	6.705418	-1.918550	-4.006625
H	8.421315	-0.086658	-4.055411
H	8.270685	1.814061	-2.422413
H	6.420919	1.888437	-0.748632
C	5.369160	1.188884	1.978683
C	5.640583	2.177355	2.936082
C	4.984421	3.421208	2.872932
C	4.064019	3.681706	1.844503
C	3.798396	2.704977	0.868490
H	5.862251	0.206478	2.051569
H	6.355442	1.968180	3.747021
H	5.183727	4.187331	3.638516
H	3.520940	4.637609	1.803104
H	3.069266	2.940884	0.080460
C	4.964197	-2.383992	0.729509
C	4.816270	-3.506870	1.563314
C	3.654441	-3.663546	2.340735
C	2.630530	-2.699638	2.288505
C	2.765357	-1.576396	1.456258
H	5.880008	-2.262332	0.130775
H	5.618138	-4.260384	1.606686
H	3.547309	-4.542153	2.996358
H	1.714017	-2.804052	2.888698
H	1.952363	-0.834894	1.437492
C	2.569940	0.579527	-1.162322
H	2.786409	1.600824	-1.543386
H	1.781773	0.693537	-0.386259

F	0.737184	1.182825	5.532310
F	-1.530010	-0.353960	5.289323
F	-2.672118	-0.736447	2.887279
C	-3.049966	-2.249266	0.313945
C	-4.040027	-3.238121	0.446796
C	-5.379067	-2.907021	0.177979
C	-5.699468	-1.592567	-0.203199
C	-4.662300	-0.646731	-0.324508
F	-3.731206	-4.503389	0.817822
F	-6.342207	-3.836072	0.292930
F	-6.979367	-1.267703	-0.460277
F	-5.042658	0.597067	-0.710061
H	1.807168	1.263781	-1.211055
H	3.289781	0.633295	-1.951571
C	3.941727	-1.024345	0.229698
F	-1.775469	-2.642170	0.600660
F	0.705117	2.001413	0.873720
F	-0.805666	3.229712	-1.810030
N	5.229310	-0.563748	0.227592
C	6.097572	-1.598649	0.561959
C	5.329492	-2.713806	0.776663
N	4.001444	-2.348990	0.565441
C	2.880902	-3.263685	0.688523
H	5.600824	-3.730023	1.076513
H	7.177677	-1.438959	0.632535
C	5.638713	0.802883	-0.035379
C	2.759848	-4.306094	-0.266136
C	1.657727	-5.173867	-0.143572
C	0.699113	-5.034700	0.880323
C	0.886787	-4.008956	1.827068
C	1.970767	-3.113318	1.766812
C	3.780623	-4.537600	-1.360253
H	1.542455	-5.985886	-0.880730
C	-0.504705	-5.935936	0.964640
C	0.153528	-3.887140	2.640229
C	2.108889	-2.047143	2.828604
C	5.566810	1.754924	1.010346
C	5.965407	3.073472	0.708613
C	6.424963	3.448759	-0.568148
C	6.508945	2.454397	-1.566035
C	6.128065	1.121652	-1.327871
C	5.081586	1.410559	2.399852
H	5.913103	3.831447	1.507452
C	6.795487	4.881842	-0.870235
H	6.884030	2.724411	-2.566923
C	6.263859	0.073427	-2.409553
H	-1.434853	-5.350766	0.822484
H	-0.475420	-6.739747	0.199374
H	-0.578292	-6.418683	1.963439
H	3.317496	-5.050020	-2.226356
H	4.242785	-3.600086	-1.728108
H	4.609849	-5.191200	-1.009860
H	7.573101	4.948118	-1.657298
H	5.908850	5.444199	-1.237046
H	7.164703	5.408894	0.032025
H	5.651055	1.979959	3.161181
H	4.012553	1.681980	2.540715
H	5.188983	0.333164	2.634855
H	7.105756	-0.622796	-2.203022
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

TSG_Bimetallic_P ^t Bu ₃	TSG_Bimetallic_PPh ₃	TSG_Bimetallic_NHC ^{mes}
E _{BP86} =-6399.718654 E _{M06} =-6396.865791	E _{BP86} =-6621.202350 E _{M06} =-6618.161122	E _{BP86} =-6509.162438 E _{M06} =-6506.015527
C 0.333313 -1.575019 -1.066209 C -1.080699 -1.529238 -1.019106 C -1.940586 -1.941435 -2.196868 C -1.739857 -1.176877 0.191485 O -0.970374 -0.963906 1.286956 C -1.618050 -0.854362 2.565629 O -3.011333 -1.112471 0.340987 C 1.184390 0.257280 -1.756944 C 2.511459 -0.283824 -1.722680 O 3.105945 -0.922636 -2.756340 C 3.194910 -0.362215 -0.474478 O 3.124505 -0.392208 -0.598370 C 0.426109 0.426803 -3.062197 H -0.651263 0.576316 -2.853293 H 0.504172 -0.474016 -3.700167 H 0.763640 1.292752 -3.674306 C 0.878038 1.243861 -0.609041 H 4.193171 -0.644484 -4.461740 H 3.120648 0.742686 -0.405900 H 2.417536 -0.778878 -4.746172 H 0.887563 -1.558533 -0.115653 H 0.791519 -2.195870 -1.853751 H -2.725983 -2.664182 -1.890526 H -1.320878 -2.434814 -2.971658 H -2.468876 -1.094126 -2.680784 H -2.244723 -1.745582 2.771602 H -0.795149 -0.786025 3.299714 H -2.254284 0.051334 2.610127 Al -4.788624 -0.847263 -0.022542 C -5.469202 0.317514 1.492124 C -5.049709 0.273270 -1.696258 C -5.514551 -2.714756 -0.089466 Al 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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	-2.482959
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



Zwitterion

Zwitterion_P ^t Bu ₃	Zwitterion_PPh ₃	Zwitterion_NHC ^{mes}
E _{BP86} =-3627.043596 E _{M06} =-3625.399770	E _{BP86} =-3848.533001 E _{M06} =-3846.697377	E _{BP86} =-3736.487259 E _{M06} =-3734.556750
C 1.232394 0.725568 -2.657440 C 0.167328 -0.027931 -2.217458 O -0.658943 -0.602752 -3.155265 C -0.938859 -1.996344 -3.005316 O -0.122706 -0.234889 -0.937779 C 1.472200 0.978018 -4.126912 H 1.256653 2.038773 -4.398758 H 0.820784 0.337423 -4.749882 H 2.527150 0.790576 -4.443003 C 2.038747 1.524623 -1.662510 H -1.766002 -2.231222 -3.701835 H -1.246960 -2.255487 -1.972691 H -0.4048507 -2.609346 -3.279930 Al -1.603037 -0.048142 0.127349 C -1.708934 1.893408 0.741063 C -3.255655 -0.578187 -0.908678 C -1.190204 -1.270345 1.696377 C -4.048207 -1.704921 -0.646919 C -5.189180 -2.039450 -1.402427 C -5.560437 -1.210907 -2.476443 C -4.796330 -0.067801 -2.778929 C -3.669312 0.216694 -1.988718 F -3.735126 -2.543141 0.370590 F -5.920908 -3.130881 -1.118728 F -6.641850 -1.508680 -3.211654 F -5.156988 0.722532 -3.803960 F -2.966502 1.331784 -2.304919 C -0.579401 2.563896 1.220865 C -0.556640 3.908541 1.624588 C -1.755087 4.641857 1.578126 C -2.931383 4.015718 1.127914 C -2.883729 2.663654 0.733370 F 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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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