

Supporting Information

The Curious Case of Co-Planarity in Di-nuclear Triel Complexes: A Density Functional Investigation

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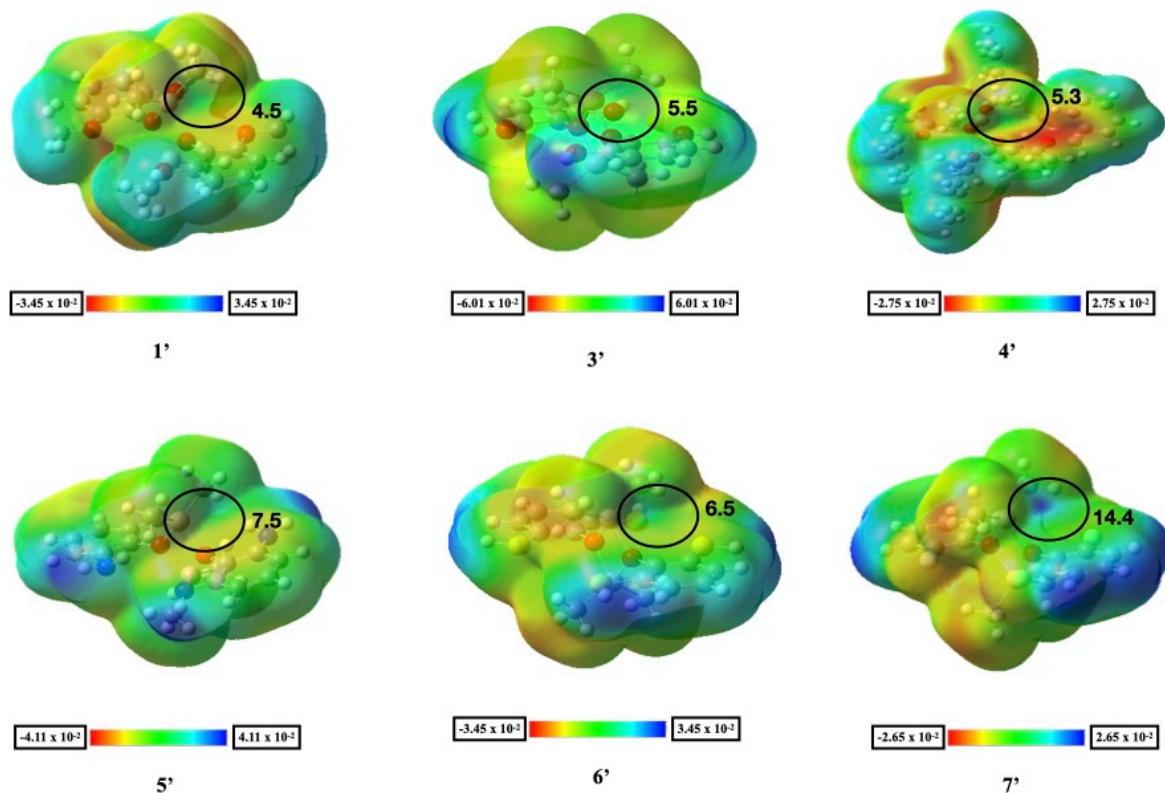
Table S1 : Interaction energy and Triel bond length calculated for di-nuclear Al complex (1) at three functionals and def2TZVP basis set.

| S.No | Method | Interaction energy (kcal/mol) | Triel Bond length (Å) |
|------|------------------|-------------------------------|-----------------------|
| 1 | B97D/def2tzvp | -11.6 | 2.60 |
| 2 | M06/def2tzvp | -11.7 | 2.59 |
| 3 | PBE0-D3/def2tzvp | -12.0 | 2.59 |

Table S2 : Topological parameters for triel bond (Tr..X) and C-H..X interaction present in di-nuclear complexes and their respective rotamers.

| S.No | Metal | Substituent | Tr..X | | | C-H..X | | |
|------|-------|------------------|-------------------------------------|--------------------------|--------------------------|-------------------------------------|--------------------------|--------------------------|
| | | | $\Delta^2\rho \times 10^{-2}$ (a.u) | $V \times 10^{-2}$ (a.u) | $K \times 10^{-2}$ (a.u) | $\Delta^2\rho \times 10^{-2}$ (a.u) | $V \times 10^{-2}$ (a.u) | $K \times 10^{-2}$ (a.u) |
| 1 | Al | -OMe | 3.30 | 0.85 | 0.79 | 0.21 | 3.0 | 1.9 |
| 2 | Al | -OEt | 3.30 | 0.90 | 0.28 | 0.38 | 9.0 | 1.7 |
| 3 | Al | -OH | 3.00 | 0.69 | 0.40 | 0.37 | 9.3 | 2.1 |
| 4 | Al | -OPh | 6.60 | 1.70 | 0.52 | 0.38 | 9.8 | 2.6 |
| 5 | Al | -NH ₂ | 4.60 | 1.50 | 0.19 | 0.38 | 9.8 | 3.9 |
| 6 | Al | -SH | 2.20 | 1.00 | 0.24 | 0.35 | 8.7 | 1.7 |
| 7 | Al | -F | 0.99 | 0.30 | 0.28 | 0.36 | 8.9 | 3.9 |
| 8 | Al | -Cl | 0.30 | 0.74 | 0.87 | 0.40 | 7.5 | 2.4 |
| 9 | B | -OMe | 5.4 | 0.65 | 0.56 | 2.5 | 0.35 | 0.14 |
| 10 | Ga | -OMe | 4.6 | 0.74 | 0.89 | 2.2 | 0.31 | 0.12 |
| 11 | In | -OMe | 4.9 | 1.24 | 0.95 | 2.0 | 0.28 | 0.13 |
| 12 | Tl | -OMe | 6.2 | 1.30 | 0.76 | 2.8 | 0.41 | 0.15 |

Figure S1: (a) MEP surface plots of rotamer di-nuclear Al complexes and the magnitude of sigma-hole present on trial atom in kcal/mol.



(b) MEP surface plots of rotamer di-nuclear complexes of B, Ga, In & Tl (9'-12') and the magnitude of sigma-hole present on trial atom in kcal/mol.

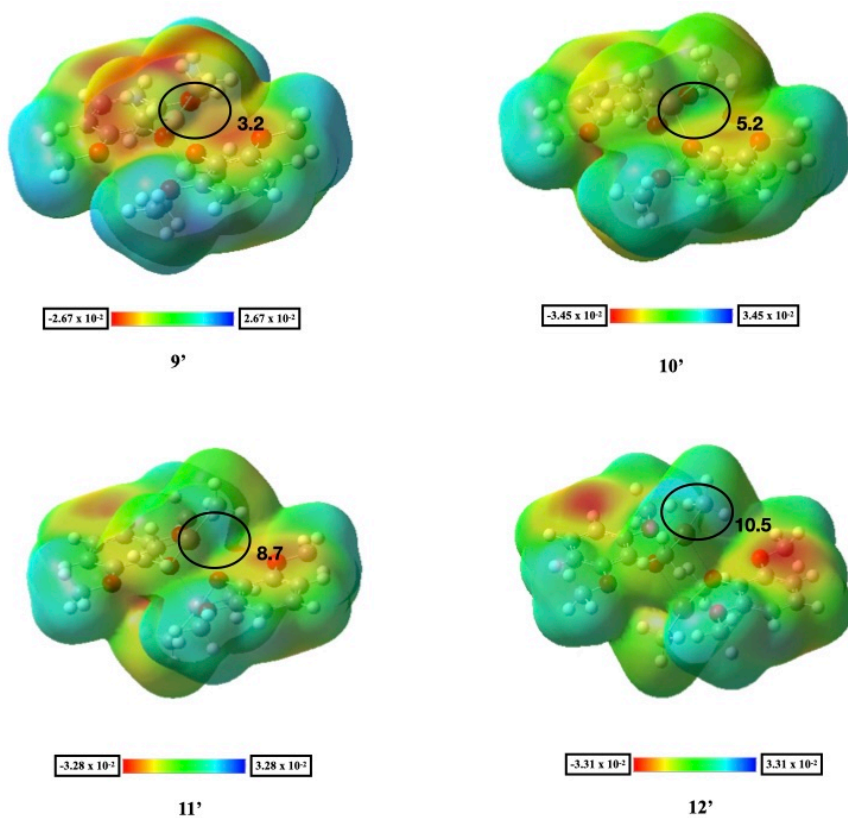
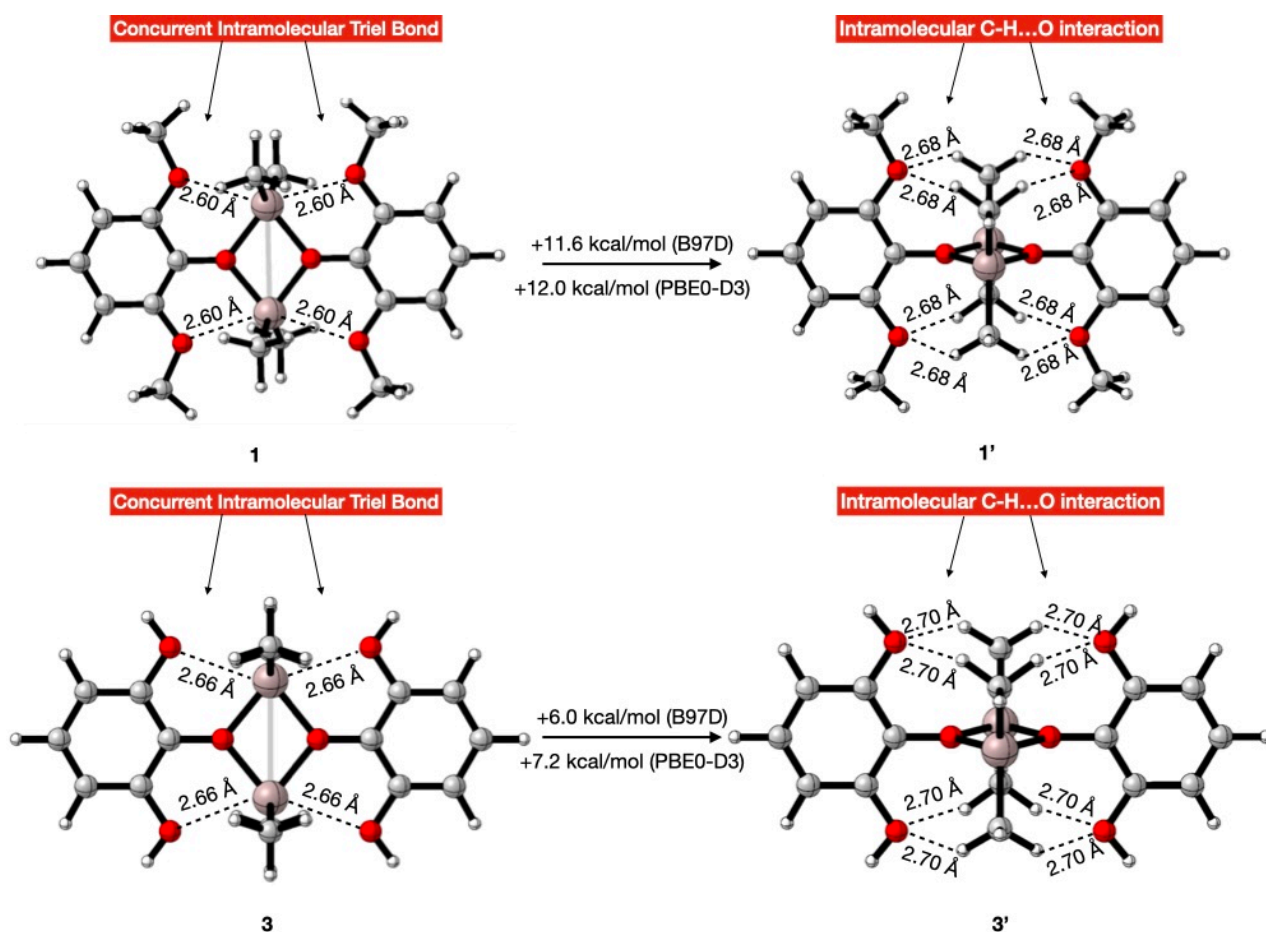
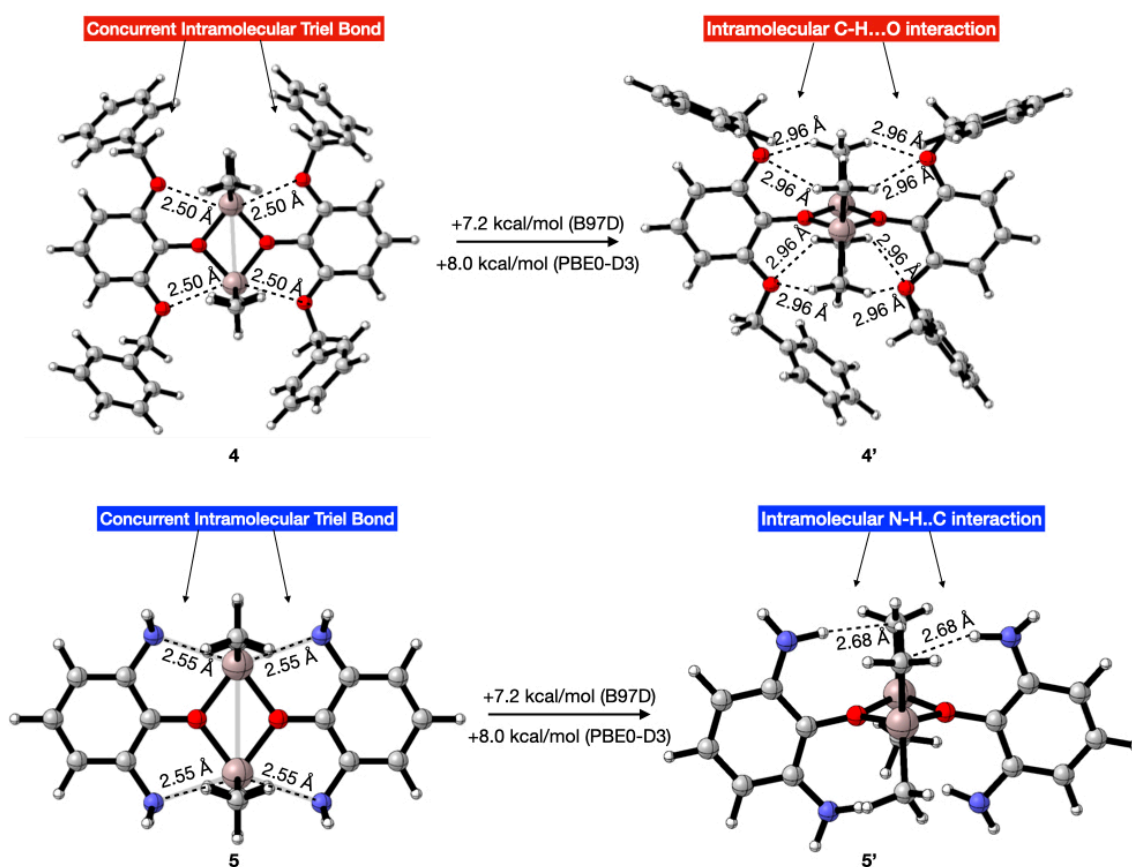


Figure S2: (a) Optimized Structures of d-nuclear Al complexes (**1** and **3**) and its rotamer (**1'** and **3'**)



(b) Optimized Structures of d-nuclear Al complexes (**4** and **5**) and its rotamer (**4'** and **5'**)



(c) Optimized Structures of d-nuclear Al complexes (**6 and 7**) and its rotamer (**6' and 7'**)

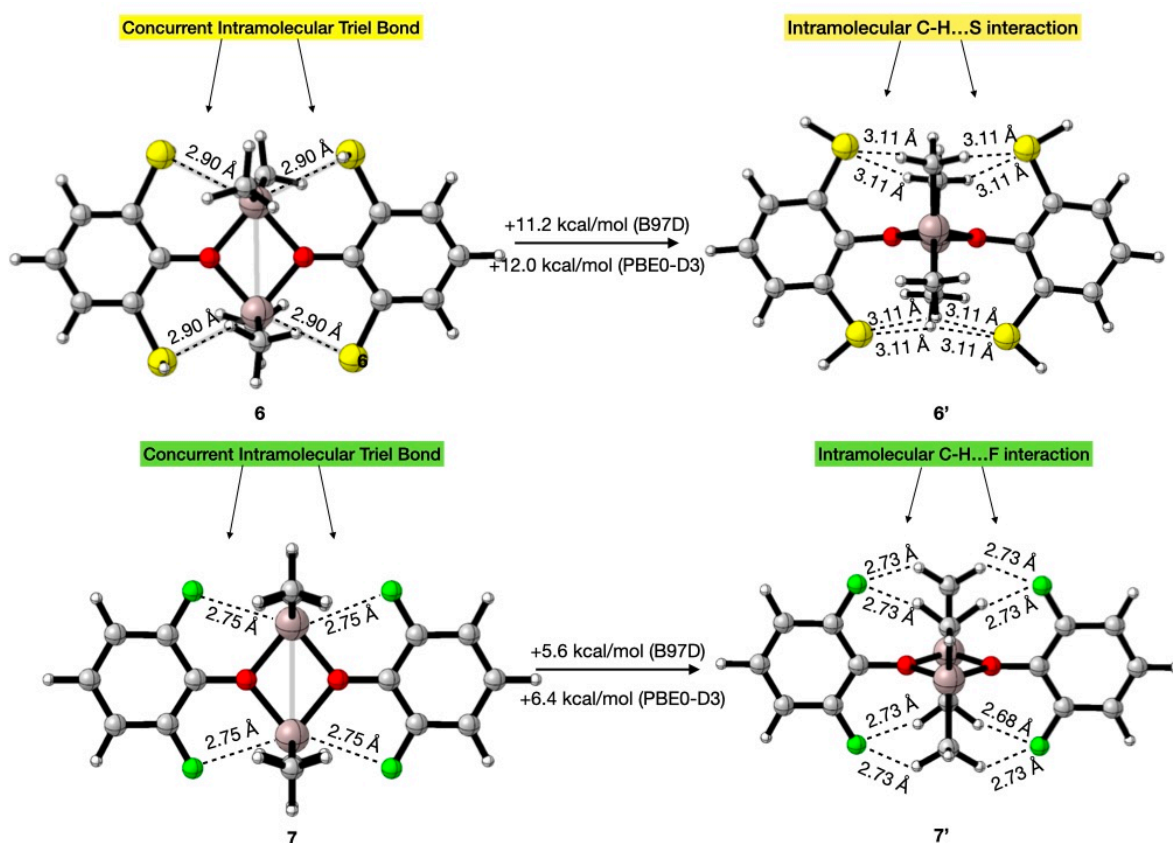
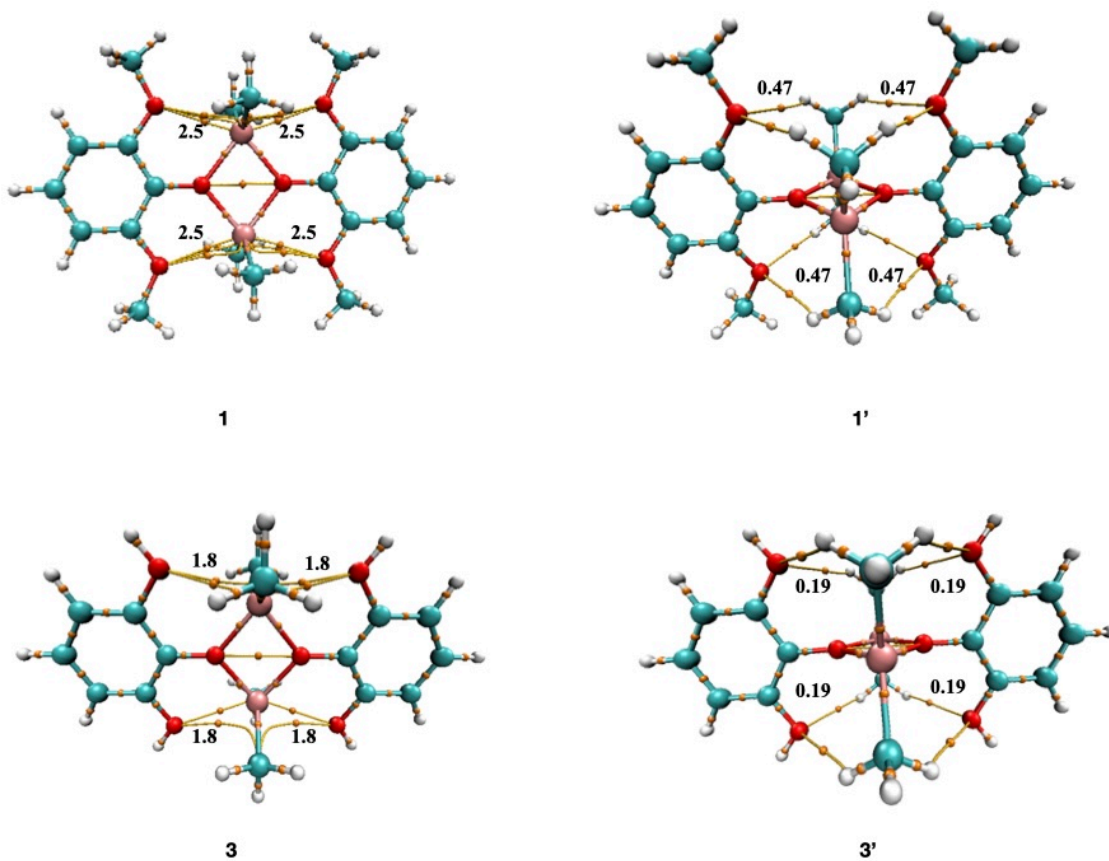
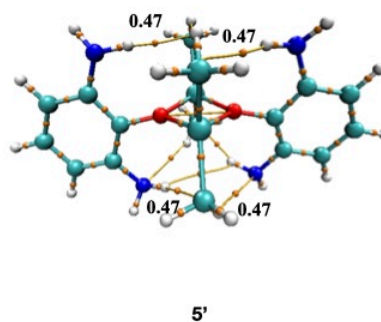
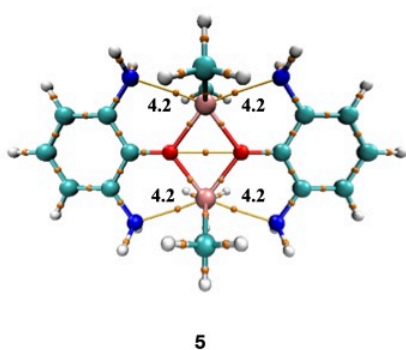
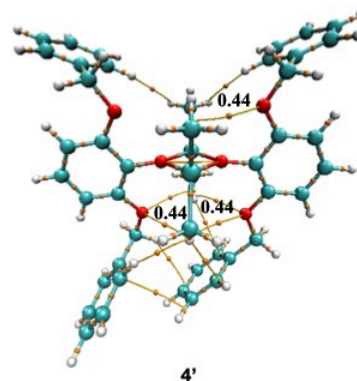
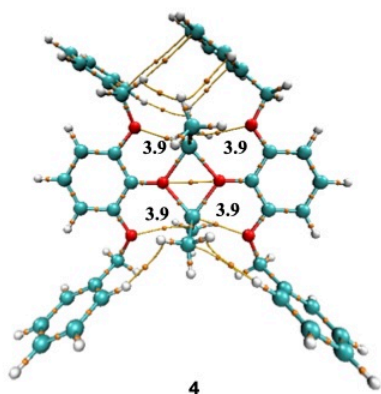


Figure S3 : (a) AIM molecular graphs of di-nuclear complexes of Al (**1 and 3**) and its corresponding rotamer (**1' and 3'**) with ρ at BCP provided



(b) AIM molecular graphs of di-nuclear complexes of Al (4 and 5) and its corresponding rotamer (4' and 5') with ρ at BCP provided



(c) AIM molecular graphs of di-nuclear complexes of Al (6 and 7) and its corresponding rotamer (6' and 7') with ρ at BCP provided

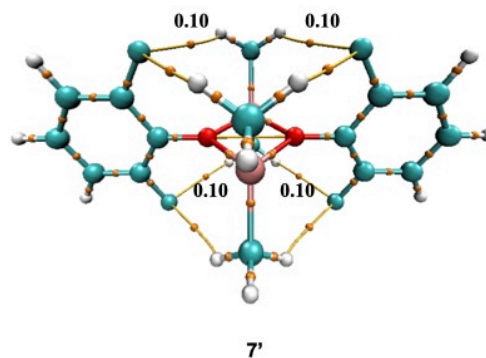
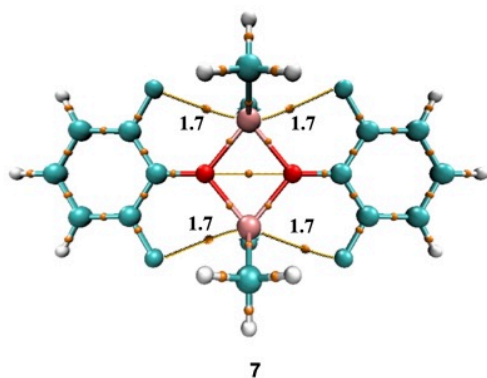
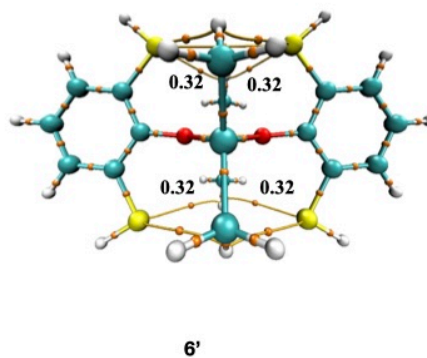
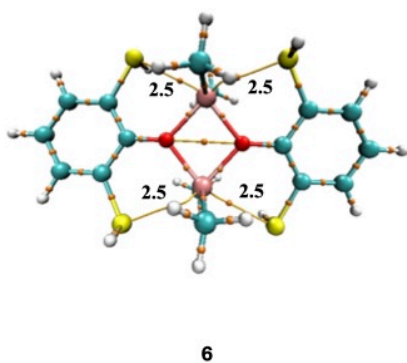
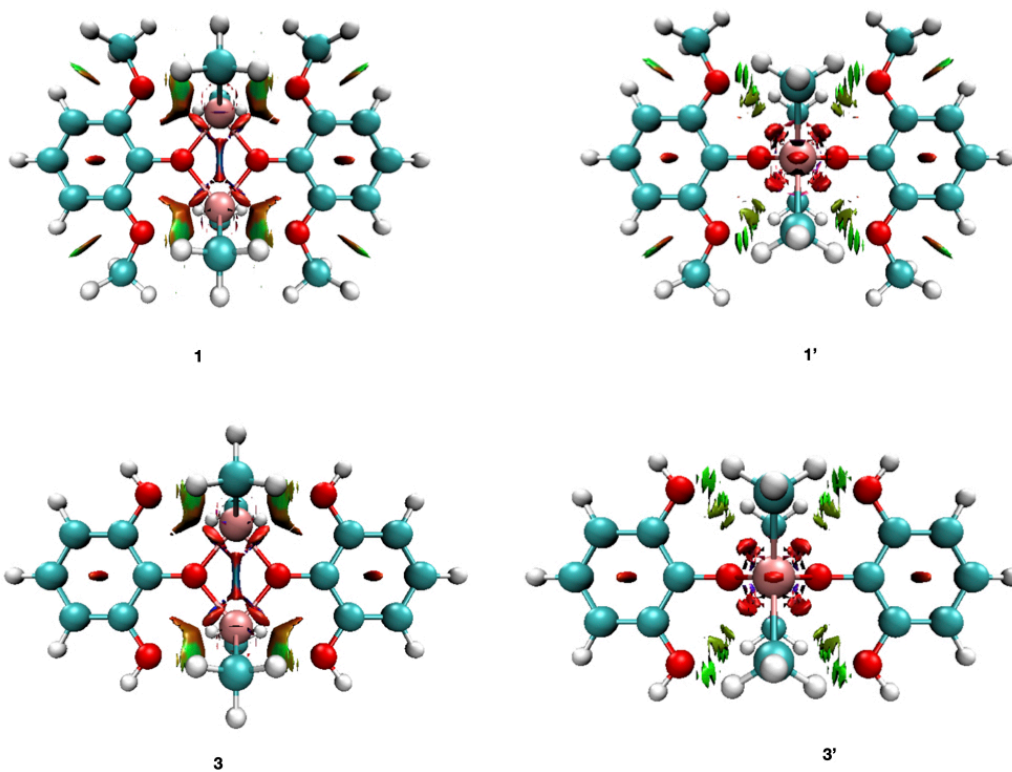
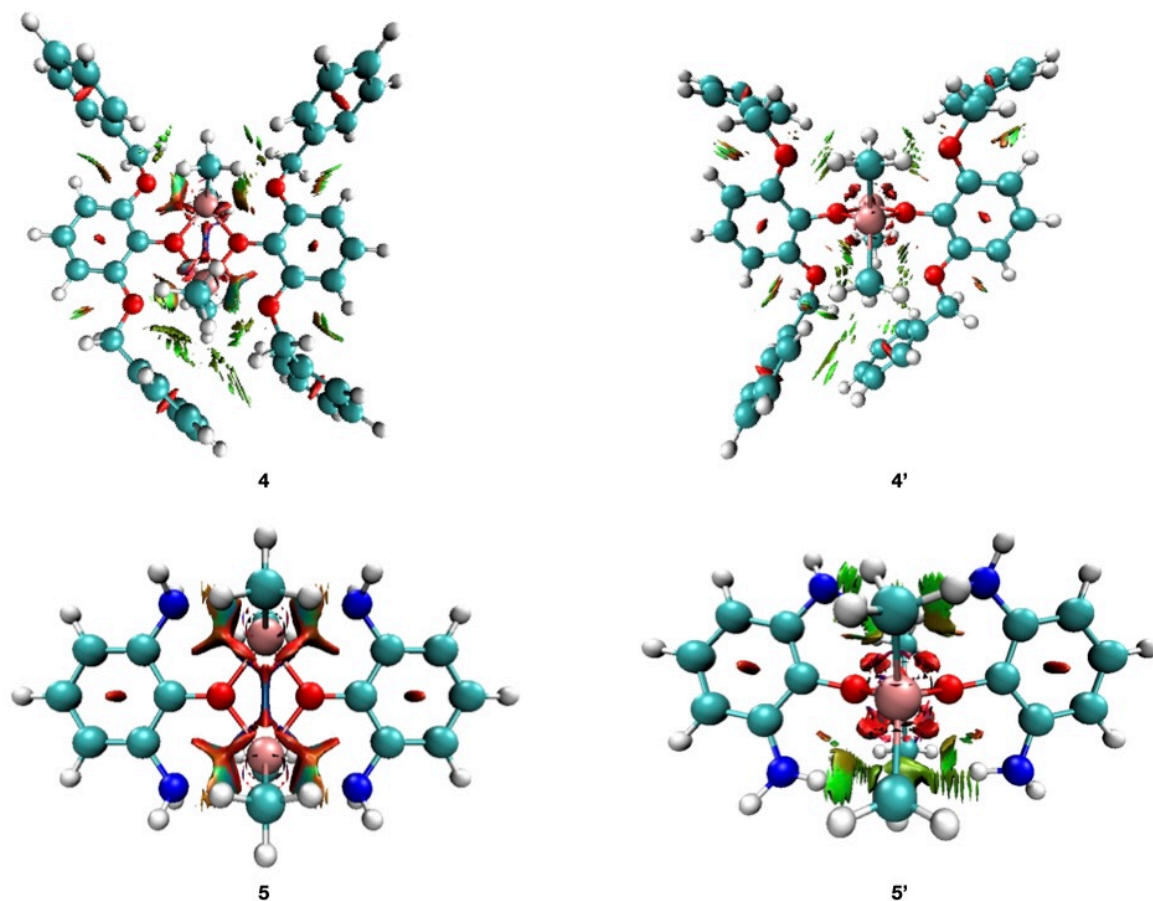


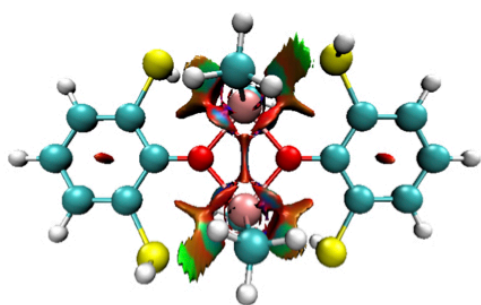
Figure S4 : (a) NCIplot of di-nuclear complexes of Al (**1** and **3**) and its corresponding rotamer (**1'** and **3'**)



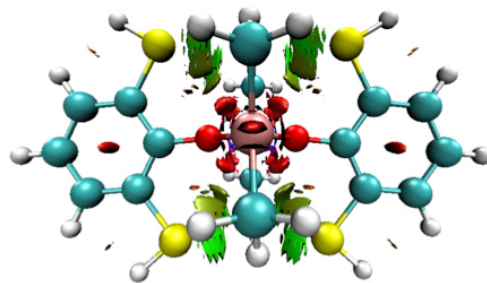
(b) NCIplot of di-nuclear complexes of Al (**4** and **5**) and its corresponding rotamer (**4'** and **5'**)



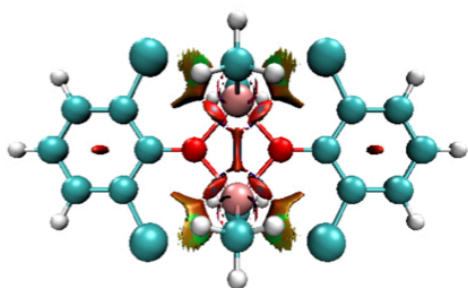
(c) NCIPlot of di-nuclear complexes of Al (6 and 7) and its corresponding rotamer (6' and 7')



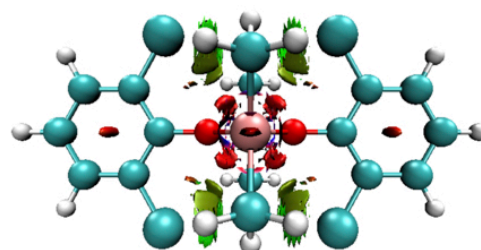
6



6'



7



7'

Reaction Co-ordinates

[(Al)Me₂(2,6-(OMe)₂C₆H₃O)]₂ (1)

0,1

| | | | |
|----|---------------|---------------|---------------|
| C | 5.3609392876 | 0.000185093 | -0.0003598189 |
| C | 4.6737932416 | 1.2152587057 | -0.0003285182 |
| C | 3.2748737016 | 1.2093103902 | -0.0001452677 |
| C | 2.5588963479 | 0.000152635 | 0.0000191203 |
| C | 3.2748974675 | -1.2089846366 | -0.0000462515 |
| C | 4.6738182383 | -1.2149024914 | -0.000231233 |
| H | 6.4514500135 | 0.0001968516 | -0.0005126008 |
| H | 5.2226460894 | 2.1556984192 | -0.0004602953 |
| H | 5.2226905385 | -2.1553304414 | -0.0002821118 |
| O | 1.1987369662 | 0.0000855771 | 0.0001922669 |
| O | 2.4759517037 | 2.3207682743 | -0.0001570796 |
| O | 2.4759754877 | -2.3204438871 | 0.0000662588 |
| C | 3.090113037 | -3.6045730065 | -0.000124895 |
| H | 2.2664930307 | -4.3271166316 | -0.0000461753 |
| H | 3.707713417 | -3.7494464992 | -0.9014999471 |
| H | 3.7079965166 | -3.7495775288 | 0.9010347744 |
| C | 3.0900917242 | 3.6048976788 | -0.0003920026 |
| H | 3.707720573 | 3.7497227483 | -0.9017548025 |
| H | 2.2664766091 | 4.3274466136 | -0.0003740498 |
| H | 3.7079470012 | 3.7499393421 | 0.9007806709 |
| Al | -0.0001102747 | 1.5145160599 | 0.0003399021 |
| Al | 0.0001122542 | -1.5145142945 | 0.0002930718 |
| O | -1.1987367718 | -0.0000839189 | 0.0004365185 |
| C | -2.5588959711 | -0.0001515489 | 0.0001817986 |
| C | -3.274898404 | 1.2089850503 | 0.0000506061 |
| C | -3.2748722267 | -1.2093099749 | 0.0000006474 |
| C | -4.6738189696 | 1.2149015515 | -0.0002567742 |
| C | -4.6737915414 | -1.2152596963 | -0.0003021108 |
| C | -5.3609388777 | -0.0001867215 | -0.0004202745 |
| H | -5.22269157 | 2.1553295233 | -0.0003781529 |
| H | -5.2226428746 | -2.1557004799 | -0.0004549125 |
| H | -6.4514495505 | -0.0001995759 | -0.0006728674 |
| O | -2.4759796511 | 2.3204462645 | 0.0002020471 |
| O | -2.4759508282 | -2.3207679526 | 0.0001156544 |
| C | -3.0901232646 | 3.6045723196 | -0.0002347669 |
| H | -2.2665070047 | 4.3271201902 | -0.0001149649 |
| H | -3.7075900539 | 3.7493356718 | -0.9017190223 |
| H | -3.7081421676 | 3.7496800647 | 0.9008154649 |
| C | -3.0900938712 | -3.6048957691 | -0.0002588857 |
| H | -3.7080891062 | -3.7499670478 | 0.900812974 |
| H | -3.7075838942 | -3.7496874049 | -0.9017222829 |
| H | -2.2664806979 | -4.3274468797 | -0.0001357281 |
| C | 0.0001340252 | -2.3403339957 | -1.7937426976 |
| H | 0.8880187824 | -2.0468479213 | -2.3752263705 |

| | | | |
|---|---------------|---------------|---------------|
| H | -0.0001406511 | -3.4423875083 | -1.743532699 |
| H | -0.8874903551 | -2.0464195418 | -2.3754101105 |
| C | -0.0003867119 | 2.3403949182 | -1.7936674941 |
| H | -0.888143883 | 2.0465815672 | -2.3751839125 |
| H | -0.0005499112 | 3.4424466606 | -1.7434205874 |
| H | 0.8873652628 | 2.0468455655 | -2.3753214388 |
| C | -0.0000705422 | 2.3403684647 | 1.7943630747 |
| C | 0.0003320549 | -2.3404262474 | 1.7942875264 |
| H | -0.8878199304 | 2.0466924015 | 2.3759563669 |
| H | 0.8876929166 | 2.0466586723 | 2.3759190032 |
| H | -0.0000522943 | 3.442421977 | 1.744143666 |
| H | -0.8875692109 | -2.0471007913 | 2.3758239779 |
| H | 0.0007763513 | -3.4424778729 | 1.7440309877 |
| H | 0.8879434223 | -2.0464039853 | 2.3759197236 |

[(Al)Me₂(2,6-(OMe)₂C₆H₃O)]₂ (1')

0,1

| | | | |
|----|-----------|-----------|-----------|
| C | 5.367072 | 0.000246 | 0.000011 |
| C | 4.685303 | 1.216415 | -0.000053 |
| C | 3.282448 | 1.219284 | -0.000044 |
| C | 2.576995 | 0.000002 | 0.000014 |
| C | 3.282654 | -1.219160 | 0.000070 |
| C | 4.685510 | -1.216038 | 0.000076 |
| H | 6.458161 | 0.000338 | 0.000010 |
| H | 5.241282 | 2.152210 | -0.000111 |
| H | 5.241655 | -2.151735 | 0.000132 |
| O | 1.200760 | -0.000085 | 0.000011 |
| O | 2.504988 | 2.339703 | -0.000140 |
| O | 2.505414 | -2.339740 | 0.000160 |
| C | 3.163520 | -3.602386 | 0.000292 |
| H | 2.363478 | -4.351401 | 0.000368 |
| H | 3.787461 | -3.733103 | -0.899775 |
| H | 3.787454 | -3.732919 | 0.900390 |
| C | 3.162829 | 3.602485 | -0.000307 |
| H | 3.786732 | 3.733126 | -0.900412 |
| H | 2.362629 | 4.351330 | -0.000397 |
| H | 3.786751 | 3.733355 | 0.899751 |
| Al | -0.000014 | -0.000012 | 1.467605 |
| Al | 0.000013 | -0.000028 | -1.467601 |
| O | -1.200760 | 0.000061 | -0.000007 |
| C | -2.576994 | 0.000001 | -0.000013 |
| C | -3.282627 | 1.219178 | 0.000033 |
| C | -3.282473 | -1.219266 | -0.000059 |
| C | -4.685483 | 1.216086 | 0.000041 |
| C | -4.685327 | -1.216367 | -0.000068 |
| C | -5.367071 | -0.000184 | -0.000014 |
| H | -5.241609 | 2.151794 | 0.000089 |

| | | | |
|---|-----------|-----------|-----------|
| H | -5.241327 | -2.152150 | -0.000117 |
| H | -6.458160 | -0.000253 | -0.000015 |
| O | -2.505362 | 2.339741 | 0.000119 |
| O | -2.505035 | -2.339700 | -0.000139 |
| C | -3.163440 | 3.602402 | 0.000274 |
| H | -2.363381 | 4.351399 | 0.000357 |
| H | -3.787383 | 3.733147 | -0.899787 |
| H | -3.787365 | 3.732935 | 0.900377 |
| C | -3.162902 | -3.602469 | -0.000265 |
| H | -3.786823 | -3.733298 | 0.899800 |
| H | -3.786811 | -3.733125 | -0.900363 |
| H | -2.362717 | -4.351330 | -0.000334 |
| C | 0.000442 | 1.722478 | -2.419718 |
| H | 0.886334 | 2.317024 | -2.146524 |
| H | -0.002721 | 1.602450 | -3.513810 |
| H | -0.881794 | 2.320161 | -2.141635 |
| C | -0.000009 | 1.722505 | 2.419702 |
| H | -0.883981 | 2.318697 | 2.143907 |
| H | -0.000201 | 1.602487 | 3.513800 |
| H | 0.884157 | 2.318539 | 2.144198 |
| C | -0.000059 | -1.722534 | 2.419692 |
| C | -0.000386 | -1.722560 | -2.419670 |
| H | -0.884521 | -2.318319 | 2.144595 |
| H | 0.883617 | -2.318970 | 2.143483 |
| H | 0.000660 | -1.602524 | 3.513791 |
| H | -0.886097 | -2.317251 | -2.146207 |
| H | 0.002455 | -1.602564 | -3.513767 |
| H | 0.882034 | -2.320081 | -2.141819 |

[(Al)Me₂(2,6-(OEt)₂C₆H₃O)]₂ (2)

0,1

| | | | |
|---|--------------|---------------|---------------|
| C | 5.3574532501 | 0.0011499239 | -0.0001781435 |
| C | 4.6715609540 | 1.2034210765 | -0.1768159567 |
| C | 3.2721483385 | 1.1994604724 | -0.1784176152 |
| C | 2.5596608658 | 0.0005393836 | -0.0000061201 |
| C | 3.2726857271 | -1.1980777309 | 0.1783154678 |
| C | 4.6721024952 | -1.2014174149 | 0.1765394209 |
| H | 6.4480566175 | 0.0013856306 | -0.0002444035 |
| H | 5.2249482343 | 2.1311975831 | -0.3103418422 |
| H | 5.2259087919 | -2.1289540747 | 0.3099902955 |
| O | 1.1986996177 | 0.0002586681 | 0.0000697202 |
| O | 2.4657427967 | 2.2909781525 | -0.3603845912 |
| O | 2.4667877739 | -2.2899464841 | 0.3603660183 |
| C | 3.0478894949 | -3.5964192429 | 0.5053995605 |
| H | 2.2538753232 | -4.1866800256 | 0.9836434734 |
| H | 3.8948761600 | -3.5460564022 | 1.2097518070 |
| C | 3.0462633104 | 3.5977122635 | -0.5054400428 |

| | | | |
|----|---------------|---------------|---------------|
| H | 3.8931486888 | 3.5477387854 | -1.2099406845 |
| H | 2.2519203971 | 4.1876649772 | -0.9835176884 |
| Al | -0.0000761365 | 1.4974090492 | -0.2176255346 |
| Al | 0.0004421546 | -1.4973535367 | 0.2177906339 |
| O | -1.1983825851 | -0.0001916146 | 0.0001989465 |
| C | -2.5593523922 | -0.0005029525 | 0.0000472897 |
| C | -3.2724072000 | 1.1984157346 | -0.1762001561 |
| C | -3.2718655046 | -1.1997619383 | 0.1761528504 |
| C | -4.6718257874 | 1.2017042159 | -0.1746933363 |
| C | -4.6712796025 | -1.2037446731 | 0.1743402218 |
| C | -5.3571815906 | -0.0011865097 | -0.0002542443 |
| H | -5.2256238068 | 2.1294719462 | -0.3065749168 |
| H | -5.2246573960 | -2.1317811020 | 0.3060997654 |
| H | -6.4477850605 | -0.0014518644 | -0.0003766284 |
| O | -2.4665819750 | 2.2907027690 | -0.3560395698 |
| O | -2.4655327036 | -2.2916515510 | 0.3561821582 |
| C | -3.0478196132 | 3.5974393969 | -0.4980978490 |
| H | -2.2536004929 | 4.1891122911 | -0.9742485134 |
| H | -3.8943111659 | 3.5487504034 | -1.2031654546 |
| C | -3.0461683894 | -3.5986617313 | 0.4982338666 |
| H | -3.8928052349 | -3.5503110257 | 1.2031494311 |
| H | -2.2517518439 | -4.1899191828 | 0.9745711766 |
| C | 0.0017162030 | -2.5572700952 | -1.4527863362 |
| H | 0.8892655801 | -2.3450390963 | -2.0690321548 |
| H | 0.0012285751 | -3.6421990021 | -1.2503691417 |
| H | -0.8846620993 | -2.3445313509 | -2.0705378360 |
| C | -0.0015966338 | 2.0661406454 | -2.1089718250 |
| H | -0.8905878649 | 1.6954731258 | -2.6423255089 |
| H | -0.0020021336 | 3.1647433694 | -2.2122915095 |
| H | 0.8867869825 | 1.6959424080 | -2.6436636240 |
| C | 0.0006619416 | 2.5574785956 | 1.4528546124 |
| C | -0.0004215825 | -2.0662912062 | 2.1090738556 |
| H | -0.8857356316 | 2.3445309688 | 2.0705036528 |
| H | 0.8881916343 | 2.3455693274 | 2.0692410198 |
| H | -0.0001236284 | 3.6423888842 | 1.2503357831 |
| H | -0.8899059167 | -1.6968919609 | 2.6424811558 |
| H | 0.0006894289 | -3.1649062835 | 2.2122602979 |
| H | 0.8874686974 | -1.6949560528 | 2.6437994224 |
| C | -3.4476681288 | -4.2048196779 | -0.8371229947 |
| C | 3.4488249510 | -4.2058361169 | -0.8286411358 |
| C | 3.4471801669 | 4.2072222140 | 0.8285627597 |
| C | -3.4498290954 | 4.2033021929 | 0.8372413036 |
| H | -4.2186737203 | 3.6013297174 | 1.3401111324 |
| H | -2.5786070379 | 4.2753720121 | 1.5018412220 |
| H | -3.8535958444 | 5.2144121113 | 0.6791334760 |
| H | 2.5756266585 | 4.2801101505 | 1.4926349599 |
| H | 4.2163801460 | 3.6072373433 | 1.3332599782 |
| H | 3.8500633535 | 5.2183157144 | 0.6681134792 |

| | | | |
|---|---------------|---------------|---------------|
| H | -4.2167114546 | -3.6032512033 | -1.3401714492 |
| H | -2.5763072483 | -4.2765384922 | -1.5015777548 |
| H | -3.8509890364 | -5.2161043410 | -0.6789947219 |
| H | 2.5771883724 | -4.2790865930 | -1.4925655195 |
| H | 4.2177095271 | -3.6055787030 | -1.3334950946 |
| H | 3.8521223276 | -5.2167682707 | -0.6682153161 |

[(Al)Me₂(2,6-(OEt)₂C₆H₃O)]₂ (2')

0,1

| | | | |
|----|---------------|---------------|---------------|
| C | 5.3640743092 | 0.0014554344 | 0.0003028323 |
| C | 4.684744605 | -1.1923494436 | 0.2368905679 |
| C | 3.281520162 | -1.1980469464 | 0.2420787814 |
| C | 2.5784621314 | -0.0001396128 | 0.0002706837 |
| C | 3.2801552894 | 1.1985717769 | -0.2415459732 |
| C | 4.6833858922 | 1.1944831469 | -0.2363138896 |
| H | 6.4552771734 | 0.0020810385 | 0.0003267446 |
| H | 5.2457294308 | -2.1077505425 | 0.4144332403 |
| H | 5.2433423963 | 2.1105203803 | -0.4138360088 |
| O | 1.2008534683 | -0.0009093561 | 0.0002525876 |
| O | 2.4969147586 | -2.2873821512 | 0.4827499617 |
| O | 2.4942954901 | 2.2869808598 | -0.4822645456 |
| C | 3.1121531303 | 3.5675567856 | -0.6834006139 |
| H | 2.3407680886 | 4.1527439423 | -1.2039258284 |
| H | 3.9725978647 | 3.4724687549 | -1.3674174792 |
| C | 3.1162360675 | -3.5674454445 | 0.6826748847 |
| H | 3.9765892503 | -3.4720488689 | 1.3667650299 |
| H | 2.345527326 | -4.1539957095 | 1.2026625611 |
| Al | -0.0001392726 | 0.2544164756 | 1.443908041 |
| Al | 0.0001027125 | -0.2563445352 | -1.4435749904 |
| O | -1.2009054031 | -0.0003960434 | -0.0000285953 |
| C | -2.5785090821 | 0.0000250816 | -0.0001485327 |
| C | -3.2812932615 | -1.1978478477 | 0.2426519502 |
| C | -3.2804656663 | 1.1983672837 | -0.2430102796 |
| C | -4.6845201115 | -1.1924872937 | 0.2373653403 |
| C | -4.6836940431 | 1.1939626092 | -0.2378097227 |
| C | -5.3641128122 | 0.0009698951 | -0.0002356769 |
| H | -5.2453120622 | -2.1078707653 | 0.4156100106 |
| H | -5.2438590309 | 2.1097253074 | -0.4160906985 |
| H | -6.4553157459 | 0.0013423722 | -0.0002648349 |
| O | -2.4964070921 | -2.2867632785 | 0.4842517429 |
| O | -2.4948419379 | 2.2867738916 | -0.4845653258 |
| C | -3.1153596896 | -3.5666980607 | 0.6860998809 |
| H | -2.3445325982 | -4.1522179825 | 1.2070784219 |
| H | -3.9758166068 | -3.4704951679 | 1.3699426231 |
| C | -3.112956787 | 3.5671789704 | -0.6859979149 |
| H | -3.9734848962 | 3.4717623226 | -1.3698611311 |
| H | -2.3417539849 | 4.1523558231 | -1.2068080121 |

| | | | |
|---|---------------|---------------|---------------|
| C | 0.001617747 | 1.2609414267 | -2.6946703225 |
| H | 0.8884372001 | 1.8926853204 | -2.5309287925 |
| H | -0.0007553131 | 0.9441103205 | -3.7486811227 |
| H | -0.8817773584 | 1.8967222111 | -2.5281183777 |
| C | -0.0004997786 | 2.1190344806 | 2.0757841322 |
| H | -0.8845788202 | 2.6540679255 | 1.6962095211 |
| H | -0.0008366667 | 2.1970369521 | 3.1735990968 |
| H | 0.8836778501 | 2.6542651837 | 1.6967373819 |
| C | 0.0001256088 | -1.2635178444 | 2.6942212482 |
| C | -0.001725901 | -2.1213109991 | -2.0744414983 |
| H | -0.8851924645 | -1.8970203851 | 2.5291984893 |
| H | 0.8850411301 | -1.897379464 | 2.5283665393 |
| H | 0.0006791031 | -0.9472022267 | 3.7483910076 |
| H | -0.889718203 | -2.6534543107 | -1.699937849 |
| H | 0.0041728602 | -2.1999403143 | -3.1721973502 |
| H | 0.8785049322 | -2.6589996808 | -1.6897551603 |
| C | -3.5007441025 | 4.2378451919 | 0.623489697 |
| C | 3.5000231186 | 4.2379365107 | 0.6262130755 |
| C | 3.5048477131 | -4.2361263971 | -0.6275916755 |
| C | -3.5036009398 | -4.2375215981 | -0.6231712046 |
| H | -4.250005014 | -3.6498920156 | -1.174696362 |
| H | -2.6210373398 | -4.3616436834 | -1.2657013505 |
| H | -3.9287312952 | -5.2321165287 | -0.4220483005 |
| H | 2.6224368723 | -4.3594756693 | -1.2704829058 |
| H | 4.2511729849 | -3.6474327536 | -1.1780845532 |
| H | 3.9302114727 | -5.2309208457 | -0.4279564071 |
| H | -4.2475405886 | 3.6505352776 | 1.1748216613 |
| H | -2.6181100422 | 4.3611616118 | 1.2660794769 |
| H | -3.9252067729 | 5.2327900757 | 0.422688254 |
| H | 2.617458184 | 4.3610024016 | 1.268944353 |
| H | 4.2469534421 | 3.6505834176 | 1.1773157923 |
| H | 3.9243429189 | 5.2329813078 | 0.4256016734 |

[(Al)Me₂(2,6-(OH)₂C₆H₃O)]₂ (3)

0,1

| | | | |
|---|---------------|---------------|---------------|
| C | -5.3874897087 | 0.0000098496 | -0.0010479766 |
| C | -4.6921114715 | -1.209161252 | -0.0010022308 |
| C | -3.2952872192 | -1.2032208651 | -0.0004660998 |
| C | -2.5709550397 | -0.0000188517 | 0.0000226305 |
| C | -3.2952579303 | 1.2031973649 | -0.0000468985 |
| C | -4.6920830527 | 1.209164248 | -0.0005727171 |
| H | -6.4776458173 | 0.0000224258 | -0.0014751597 |
| H | -5.2273285223 | -2.1616544186 | -0.0013965027 |
| H | -5.2272785422 | 2.161669443 | -0.0005981563 |
| O | -1.2096132507 | -0.0000131256 | 0.0004559818 |
| O | -2.5304778502 | -2.3422655781 | -0.0004828223 |
| O | -2.5304198754 | 2.3422224874 | 0.0004730114 |

| | | | |
|----|---------------|---------------|---------------|
| Al | 0.0000173357 | -1.5090666825 | 0.0006094463 |
| Al | -0.0000165838 | 1.5090663718 | 0.0005550693 |
| O | 1.2096139731 | 0.0000132331 | 0.0009155371 |
| C | 2.5709555718 | 0.0000187836 | 0.0003809375 |
| C | 3.2952583388 | -1.2031974108 | 0.000062131 |
| C | 3.2952874434 | 1.2032208945 | -0.0000283467 |
| C | 4.6920832781 | -1.2091642403 | -0.0008141902 |
| C | 4.6921115542 | 1.2091613193 | -0.0008988321 |
| C | 5.3874898117 | -0.0000097108 | -0.001322932 |
| H | 5.2272786653 | -2.1616694719 | -0.0010610255 |
| H | 5.2273284229 | 2.1616546306 | -0.0012132671 |
| H | 6.4776457786 | -0.0000221544 | -0.0020291801 |
| O | 2.5304203416 | -2.3422226852 | 0.0006457494 |
| O | 2.5304781503 | 2.3422656268 | 0.0004886405 |
| C | 0.0001439119 | 2.3202938226 | -1.7956037872 |
| H | -0.8878464475 | 2.0227505955 | -2.3747150074 |
| H | 0.0005294784 | 3.4214876824 | -1.7460396273 |
| H | 0.8878681901 | 2.0221375787 | -2.3748126982 |
| C | 0.000359264 | -2.3203652355 | -1.7955141711 |
| H | 0.8882828429 | -2.0224661548 | -2.3745493104 |
| H | 0.000434289 | -3.4215571225 | -1.7459078591 |
| H | -0.887431815 | -2.0226075939 | -2.3748223192 |
| C | -0.0002237583 | -2.3206049087 | 1.7966124461 |
| C | -0.0002774353 | 2.3206767217 | 1.7965222639 |
| H | 0.887613483 | -2.0229421421 | 2.3758932417 |
| H | -0.8881161605 | -2.0227626296 | 2.3757179649 |
| H | -0.0003238907 | -3.4217893478 | 1.7468635936 |
| H | 0.8876937294 | 2.0232542389 | 2.3757192065 |
| H | -0.0006650004 | 3.421859008 | 1.7467308552 |
| H | -0.888035778 | 2.0226372834 | 2.3757348828 |
| H | -3.1002129739 | 3.1292910044 | 0.0000012797 |
| H | 3.1002805041 | 3.1293262854 | -0.0010641723 |
| H | 3.1002120276 | -3.1292906446 | -0.0010035516 |
| H | -3.1002812624 | -3.1293266727 | -0.0011971067 |

[(Al)Me₂(2,6-(OH)₂C₆H₃O)]₂ (3')

0,1

| | | | |
|---|--------------|---------------|---------------|
| C | 5.3812023871 | 0.0000302715 | -0.0000069865 |
| C | 4.6905365649 | -1.2103549182 | -0.000176526 |
| C | 3.2900419366 | -1.2124826483 | -0.0001582788 |
| C | 2.5770377227 | -0.0000088366 | -0.0000022919 |
| C | 3.2900098293 | 1.2124842215 | 0.0001513946 |
| C | 4.6905043072 | 1.2103970617 | 0.0001649257 |
| H | 6.4718733354 | 0.000044515 | -0.0000088381 |
| H | 5.2306328144 | -2.1603293488 | -0.0003300897 |
| H | 5.2305742099 | 2.1603863732 | 0.0003167475 |
| O | 1.201929257 | -0.0000187434 | -0.0000008253 |
| O | 2.5485653471 | -2.3614558733 | -0.0003982333 |

| | | | |
|----|---------------|---------------|---------------|
| O | 2.5484927274 | 2.3614287988 | 0.0003930776 |
| Al | 0.0000006731 | -0.0000183341 | 1.4712846876 |
| Al | -0.0000002835 | -0.0000156414 | -1.4712846259 |
| O | -1.2019284193 | 0.000000113 | 0.000000885 |
| C | -2.57703685 | 0.0000159185 | 0.0000018811 |
| C | -3.2900178757 | 1.2125032944 | -0.0001525264 |
| C | -3.2900318697 | -1.2124636425 | 0.0001581066 |
| C | -4.6905125535 | 1.2104021127 | -0.000167152 |
| C | -4.6905263112 | -1.2103499658 | 0.0001762444 |
| C | -5.3812013364 | 0.0000300208 | 0.0000053857 |
| H | -5.2305908072 | 2.1603867719 | -0.0003203282 |
| H | -5.2306142708 | -2.160329066 | 0.0003309736 |
| H | -6.4718722875 | 0.0000365364 | 0.000006788 |
| O | -2.5485191484 | 2.3614620949 | -0.0003968633 |
| O | -2.5485361748 | -2.3614220309 | 0.0004017444 |
| C | 0.0001036394 | 1.7256726394 | -2.4137943861 |
| H | 0.8839903654 | 2.3213703033 | -2.1365701243 |
| H | -0.0009490235 | 1.6087868006 | -3.5082873825 |
| H | -0.8825858025 | 2.3223831341 | -2.1349441521 |
| C | 0.0000122304 | 1.7256677818 | 2.4137983984 |
| H | -0.8832279815 | 2.321911629 | 2.1356981081 |
| H | -0.0000670603 | 1.6087793877 | 3.5082916226 |
| H | 0.8833491998 | 2.3218334109 | 2.13582586 |
| C | -0.000015791 | -1.7257215722 | 2.4137671717 |
| C | -0.0001024751 | -1.7257164981 | -2.4137714303 |
| H | -0.8834369679 | -2.3218134195 | 2.135902645 |
| H | 0.8831407398 | -2.322027654 | 2.1355357797 |
| H | 0.0002168211 | -1.6088544367 | 3.5082626341 |
| H | -0.8839481616 | -2.321442803 | -2.1364786797 |
| H | 0.0008741312 | -1.6088469387 | -3.5082662359 |
| H | 0.8826286934 | -2.3223890255 | -2.134971513 |
| H | 3.1588013331 | 3.1191438394 | 0.0005306734 |
| H | -3.1588587701 | -3.1191257954 | 0.0005425405 |
| H | -3.1588442772 | 3.1191639738 | -0.0005366462 |
| H | 3.1589052331 | -3.1191458711 | -0.0005391596 |

[(Al)Me₂(2,6-(OPh)₂C₆H₃O)]₂ (4)

0,1

| | | | |
|---|--------------|--------------|---------------|
| C | 2.1243560126 | 4.5407868076 | -0.0998576641 |
| C | 0.754046937 | 4.4692713965 | -0.3574647481 |
| C | 0.121504404 | 3.221467473 | -0.3803942943 |
| C | 0.8570311817 | 2.0456825392 | -0.1491586296 |
| C | 2.2358366987 | 2.1475544253 | 0.1046180539 |
| C | 2.8767901813 | 3.387863267 | 0.1326214288 |
| H | 2.6151743067 | 5.5143669716 | -0.0806157964 |
| H | 0.1773217311 | 5.3797660257 | -0.5113498529 |
| H | 3.9498962221 | 3.4503405477 | 0.3073993959 |
| O | 0.2615023245 | 0.8242969915 | -0.1685473342 |

| | | | |
|----|---------------|---------------|---------------|
| O | -1.2154911162 | 3.0081680518 | -0.6043757372 |
| O | 2.8466582239 | 0.9277213826 | 0.2883720607 |
| C | 4.1376121421 | 0.868380066 | 0.9053276534 |
| H | 4.1995440335 | -0.1597611788 | 1.2954897858 |
| H | 4.1689703362 | 1.5572362667 | 1.7667128085 |
| C | -2.0022489868 | 4.0707539744 | -1.1542943784 |
| H | -1.4652169127 | 4.5358772319 | -1.9989522413 |
| H | -2.8866566314 | 3.5567190855 | -1.5615935119 |
| Al | -1.5614508439 | 0.3086537584 | -0.5108454159 |
| Al | 1.1318743973 | -0.8619346392 | 0.1483285411 |
| O | -0.7078887449 | -1.3798505753 | -0.1667933583 |
| C | -1.2555610024 | -2.6218826735 | -0.2461287172 |
| C | -2.6100246497 | -2.7674966646 | -0.5915474028 |
| C | -0.4921614738 | -3.7800268337 | 0.0032502927 |
| C | -3.1967730694 | -4.0303156949 | -0.7113759552 |
| C | -1.0723860394 | -5.0483209794 | -0.1181781162 |
| C | -2.416811778 | -5.1624238786 | -0.4766512335 |
| H | -4.2525931931 | -4.1273658635 | -0.9576399016 |
| H | -0.483657271 | -5.9447858477 | 0.0681510676 |
| H | -2.8665736906 | -6.1520095601 | -0.5639917297 |
| O | -3.2567438045 | -1.5683700849 | -0.7843914271 |
| O | 0.8111690106 | -3.5402561374 | 0.3545012857 |
| C | -4.5131934873 | -1.5609771264 | -1.4773579361 |
| H | -4.612726404 | -0.5224071643 | -1.8277725544 |
| H | -4.4502946206 | -2.2112162696 | -2.366452495 |
| C | 1.6804976174 | -4.6752481044 | 0.5581411534 |
| H | 1.7235267701 | -5.2666154456 | -0.3730874226 |
| H | 1.2644738398 | -5.3096106576 | 1.3596328084 |
| C | 2.0884728435 | -1.3423698634 | -1.5127593442 |
| H | 1.9994412135 | -0.5173700316 | -2.2394850394 |
| H | 3.1612263043 | -1.5222483462 | -1.3514504877 |
| H | 1.6701711766 | -2.2419988642 | -1.9896612797 |
| C | -1.8867496507 | 0.5875323846 | -2.4414628466 |
| H | -1.8660593163 | -0.3607985344 | -3.0017967957 |
| H | -2.8616916044 | 1.0606905998 | -2.6469493095 |
| H | -1.1174849896 | 1.2418559903 | -2.8806566649 |
| C | -2.6300002126 | 0.7988008077 | 1.0755343143 |
| C | 1.4358129254 | -1.0224957173 | 2.0926586909 |
| H | -2.8615714033 | -0.0893379199 | 1.684584654 |
| H | -2.0737963536 | 1.4942721541 | 1.7234519266 |
| H | -3.5869166926 | 1.2823608496 | 0.8195283524 |
| H | 0.7314925973 | -1.7336092998 | 2.5507053417 |
| H | 2.4479109914 | -1.3687862006 | 2.3499560436 |
| H | 1.2859172594 | -0.0460905911 | 2.5819295377 |
| C | -2.4241285286 | 5.1171285374 | -0.1470377739 |
| C | -2.6919358538 | 4.7687212403 | 1.1823417812 |
| C | -2.5906181877 | 6.4474960037 | -0.5506216094 |
| C | -3.1162821321 | 5.7380611054 | 2.0919142226 |

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|---|---------------|---------------|---------------|
| H | -2.5584115999 | 3.7339171384 | 1.5014994403 |
| C | -3.0249675787 | 7.4161018675 | 0.3568711893 |
| H | -2.3720133543 | 6.7299204319 | -1.5842532159 |
| C | -3.28695219 | 7.0632709418 | 1.6825966895 |
| H | -3.3162655792 | 5.4556980848 | 3.1272765817 |
| H | -3.1485061695 | 8.4502194364 | 0.0297815209 |
| H | -3.6184441331 | 7.8199122768 | 2.3959154695 |
| C | -5.6951773271 | -1.9408216608 | -0.6154034415 |
| C | -6.7830924325 | -2.6147199298 | -1.1835314031 |
| C | -5.7397809268 | -1.5918424607 | 0.739787046 |
| C | -7.9042672746 | -2.9296322036 | -0.4127892614 |
| H | -6.7501457642 | -2.9010817152 | -2.2383967169 |
| C | -6.8558581001 | -1.9148816044 | 1.5125356543 |
| H | -4.89083335 | -1.0721747527 | 1.1866293119 |
| C | -7.9421711518 | -2.5814293184 | 0.939129078 |
| H | -8.7451518996 | -3.456862996 | -0.8672740567 |
| H | -6.8774771087 | -1.6427384777 | 2.5694641504 |
| H | -8.8139267149 | -2.8332914842 | 1.5456294417 |
| C | 5.2896747114 | 1.129597288 | -0.0375837645 |
| C | 6.5269739633 | 1.5252423973 | 0.4866469771 |
| C | 5.1636743294 | 0.9344014256 | -1.417388661 |
| C | 7.6257453796 | 1.7149722721 | -0.3532050092 |
| H | 6.6300842124 | 1.6905493287 | 1.5627263005 |
| C | 6.2605321463 | 1.1327915819 | -2.2583304502 |
| H | 4.2006104279 | 0.6306534875 | -1.8290392847 |
| C | 7.494646742 | 1.5196625346 | -1.7305170439 |
| H | 8.5838183609 | 2.0255732416 | 0.0678979673 |
| H | 6.1483542878 | 0.9839949722 | -3.3339856496 |
| H | 8.3501309697 | 1.6750290727 | -2.3902012498 |
| C | 3.0416559497 | -4.1626688123 | 0.9365372639 |
| C | 3.3782769525 | -3.9679612815 | 2.2817749127 |
| C | 3.9726001332 | -3.82400948 | -0.0537166341 |
| C | 4.6157130932 | -3.4255569994 | 2.63205668 |
| H | 2.653919899 | -4.2228231193 | 3.058590209 |
| C | 5.2074530787 | -3.2731638335 | 0.2912730122 |
| H | 3.7151327444 | -3.971981969 | -1.1041856648 |
| C | 5.5287971499 | -3.0687759309 | 1.6359896779 |
| H | 4.8634049555 | -3.2715473968 | 3.6837412179 |
| H | 5.9169345479 | -2.9944224705 | -0.4898329657 |
| H | 6.4934665908 | -2.6350290702 | 1.9064134853 |

[(Al)Me₂(2,6-(OPh)₂C₆H₃O)]₂ (4')

0,1

0,1

| | | | |
|---|--------------|--------------|---------------|
| C | 2.9307459626 | 4.0607245695 | -0.0410675811 |
| C | 3.374752124 | 2.7916761251 | 0.3296101486 |
| C | 2.4886704884 | 1.7086825242 | 0.2518165422 |
| C | 1.1714199473 | 1.9118653346 | -0.1991626728 |

| | | | |
|----|---------------|---------------|---------------|
| C | 0.7439812733 | 3.195354378 | -0.5849744491 |
| C | 1.6301354731 | 4.2781519213 | -0.49576965 |
| H | 3.6188662295 | 4.9049275368 | 0.0238186603 |
| H | 4.404305745 | 2.6419705558 | 0.6500627388 |
| H | 1.305571524 | 5.2834693462 | -0.7558907825 |
| O | 0.2995992507 | 0.847101271 | -0.2662177719 |
| O | 2.7843820884 | 0.4171786883 | 0.5812268984 |
| O | -0.545543569 | 3.2580057148 | -1.0341438686 |
| C | -1.0589816449 | 4.5260825902 | -1.4533714336 |
| H | -1.9805190302 | 4.2639012941 | -1.9959852921 |
| H | -0.3733265474 | 5.0032613837 | -2.1756053284 |
| C | 4.0299093346 | 0.1425941501 | 1.2204265571 |
| H | 4.2108165329 | 0.865100417 | 2.0361370326 |
| H | 3.8804484434 | -0.8480310437 | 1.678830811 |
| Al | -0.1576310662 | -0.2206464951 | -1.7557588526 |
| Al | -0.6243163994 | -0.0514794743 | 1.1146559358 |
| O | -1.0117918774 | -1.1649670751 | -0.3598707632 |
| C | -1.6943344286 | -2.3597743927 | -0.3917760093 |
| C | -3.0550035494 | -2.3819515981 | -0.7474803155 |
| C | -1.021726367 | -3.556769291 | -0.0786688032 |
| C | -3.7508803922 | -3.5999853988 | -0.7615937795 |
| C | -1.7215066353 | -4.7720393842 | -0.0967748529 |
| C | -3.0755348946 | -4.7748534133 | -0.4345308603 |
| H | -4.8130064034 | -3.6283817603 | -0.9962803727 |
| H | -1.2215277208 | -5.7058966709 | 0.15320019 |
| H | -3.6211152133 | -5.7197338715 | -0.4377572986 |
| O | -3.5822095097 | -1.1629666939 | -1.0674061687 |
| O | 0.3015051112 | -3.4117282065 | 0.2180153907 |
| C | -4.9204038051 | -1.1119833415 | -1.5737086485 |
| H | -4.9803317163 | -0.1184712769 | -2.0447871774 |
| H | -5.0606216667 | -1.8659379609 | -2.3680162266 |
| C | 1.0481294103 | -4.5951815265 | 0.5513257707 |
| H | 0.9839249925 | -5.3162832778 | -0.2834157418 |
| H | 0.6176004701 | -5.0649325529 | 1.4528509697 |
| C | 0.5030732626 | -0.9046164347 | 2.4741597662 |
| H | 1.3255490082 | -1.4702549925 | 2.0165673334 |
| H | 0.9409678008 | -0.1566495425 | 3.1552901219 |
| H | -0.0826987114 | -1.601192012 | 3.0964077281 |
| C | 1.4077067982 | -1.1931184678 | -2.4362852975 |
| H | 1.1110966777 | -2.0568910546 | -3.0536077377 |
| H | 2.0421387766 | -0.5528205615 | -3.0710899293 |
| H | 2.0219208633 | -1.5706095236 | -1.6058056304 |
| C | -1.4516361848 | 0.654555346 | -2.9443728945 |
| C | -2.2112616637 | 0.9864854717 | 1.6420605328 |
| H | -2.2443163783 | 1.1475764555 | -2.361923874 |
| H | -0.9713139812 | 1.4213290097 | -3.5732397011 |
| H | -1.9343812321 | -0.0680909265 | -3.6221933598 |
| H | -2.9198368071 | 0.3663911993 | 2.2155583086 |

| | | | |
|---|---------------|---------------|---------------|
| H | -1.9404196872 | 1.8334418693 | 2.2938649325 |
| H | -2.7450439239 | 1.3882893955 | 0.7670889207 |
| C | 5.2155283647 | 0.0833517677 | 0.2837508227 |
| C | 5.0496474313 | -0.1175673745 | -1.0904538572 |
| C | 6.5111618169 | 0.1596342805 | 0.8103006601 |
| C | 6.1632078282 | -0.2449871866 | -1.9231787456 |
| H | 4.0424740624 | -0.1810571629 | -1.5040156286 |
| C | 7.6250546135 | 0.0227946335 | -0.0199258054 |
| H | 6.6496296939 | 0.3244774309 | 1.8826147045 |
| C | 7.4536550761 | -0.181221937 | -1.3918495161 |
| H | 6.0195458022 | -0.398493753 | -2.9945680377 |
| H | 8.6293585875 | 0.0833839925 | 0.4039146224 |
| H | 8.3227944781 | -0.2825989 | -2.0441946419 |
| C | -5.9865945327 | -1.2512466071 | -0.5101056304 |
| C | -7.1872631031 | -1.9107835998 | -0.7973327104 |
| C | -5.8034670898 | -0.688780053 | 0.7593320939 |
| C | -8.1950602834 | -2.0035614251 | 0.1652601251 |
| H | -7.3334200733 | -2.3611525089 | -1.7831681221 |
| C | -6.8062532817 | -0.7879814739 | 1.7243787472 |
| H | -4.8658631789 | -0.1793204014 | 0.9886075266 |
| C | -8.0054837957 | -1.4430742073 | 1.4302293236 |
| H | -9.1258750829 | -2.5228793716 | -0.0705105967 |
| H | -6.6504152964 | -0.3497104073 | 2.7120457425 |
| H | -8.7884309653 | -1.5203463524 | 2.1867610746 |
| C | -1.3717857798 | 5.465498028 | -0.3098841672 |
| C | -1.2240286322 | 6.8481078 | -0.4696532807 |
| C | -1.8451371461 | 4.9657933263 | 0.9096110744 |
| C | -1.5489523204 | 7.721896189 | 0.5703424798 |
| H | -0.8447534836 | 7.2452511027 | -1.4154495425 |
| C | -2.1612887578 | 5.8372477826 | 1.9522140529 |
| H | -1.9556019353 | 3.8878130159 | 1.039446276 |
| C | -2.0162690396 | 7.2174057868 | 1.7858765797 |
| H | -1.4267562352 | 8.7981116692 | 0.4341145838 |
| H | -2.5243936905 | 5.4355303297 | 2.9001805316 |
| H | -2.262764457 | 7.8977523862 | 2.6029712593 |
| C | 2.4750503105 | -4.1883863758 | 0.7920159847 |
| C | 2.9719849316 | -4.0587760083 | 2.0936883907 |
| C | 3.3211768971 | -3.9118643894 | -0.2911296867 |
| C | 4.2965131243 | -3.6697836811 | 2.3116907645 |
| H | 2.3135413854 | -4.2566670831 | 2.9425933684 |
| C | 4.6415333118 | -3.5171467874 | -0.0773972296 |
| H | 2.9339115223 | -3.9964427846 | -1.3089928019 |
| C | 5.1332545193 | -3.400534223 | 1.2262693479 |
| H | 4.6736048934 | -3.5742080671 | 3.3316837864 |
| H | 5.2880753096 | -3.2878628161 | -0.9255642784 |
| H | 6.1654626194 | -3.0868089102 | 1.3912411909 |

[(Al)Me₂(2,6-(NH₂)₂C₆H₃O)]₂ (5)

0,1

| | | | |
|----|---------------|---------------|---------------|
| C | 5.3165026172 | 0.0002685229 | 0.0005741162 |
| C | 4.6129197808 | 1.2074140034 | 0.0016861668 |
| C | 3.217143874 | 1.2191162267 | 0.0014215162 |
| C | 2.5087906596 | -0.0000121187 | -0.0001427828 |
| C | 3.2173693301 | -1.219014156 | -0.0012677936 |
| C | 4.6131488784 | -1.2070099375 | -0.0008478634 |
| H | 6.4070009786 | 0.000372082 | 0.0008345004 |
| H | 5.1501120184 | 2.1590174421 | 0.002884021 |
| H | 5.1505287736 | -2.1585080565 | -0.0017401349 |
| O | 1.1705818361 | -0.0000704176 | -0.0005381701 |
| Al | 0.0000919069 | 1.5631231647 | -0.0004544047 |
| Al | -0.0000857795 | -1.5631977765 | -0.0005015773 |
| O | -1.1705827537 | 0.0000033483 | -0.0011915833 |
| C | -2.5087962122 | -0.000006707 | -0.000430326 |
| C | -3.2172809721 | 1.2190511067 | -0.00117351 |
| C | -3.2172607028 | -1.2190795352 | 0.0012763975 |
| C | -4.6130605104 | 1.2071658673 | 0.0002424894 |
| C | -4.6130354526 | -1.2072544707 | 0.002561799 |
| C | -5.3165157459 | -0.0000504572 | 0.0021828528 |
| H | -5.1503598089 | 2.1587096096 | -0.0002664108 |
| H | -5.1503110487 | -2.1588107488 | 0.0039603414 |
| H | -6.4070134858 | -0.0000612534 | 0.0032847663 |
| C | -0.0011995175 | -2.2692227922 | -1.861598674 |
| H | 0.8811560571 | -1.9366334197 | -2.4336678092 |
| H | -0.0003630663 | -3.3735050511 | -1.8857739189 |
| H | -0.8851830003 | -1.9380235584 | -2.4319411323 |
| C | 0.0016869537 | 2.2693425107 | -1.8614562714 |
| H | -0.880497541 | 1.9368597139 | -2.4338537214 |
| H | 0.0009212049 | 3.3736275447 | -1.8854700418 |
| H | 0.8858538636 | 1.9382006377 | -2.4315389666 |
| C | -0.0019007001 | 2.268371473 | 1.8609003323 |
| C | 0.0014850036 | -2.2686352222 | 1.8607770934 |
| H | -0.8861567811 | 1.9368885092 | 2.4306386309 |
| H | 0.8802184589 | 1.9356567378 | 2.433269213 |
| H | -0.0012094744 | 3.3726444162 | 1.8854782284 |
| H | -0.8808374846 | -1.9360404565 | 2.4328941791 |
| H | 0.0008050721 | -3.3729117378 | 1.8851953291 |
| H | 0.8855484451 | -1.9371990333 | 2.4308474632 |
| N | 2.4085865446 | 2.4125348641 | 0.0025979086 |
| H | 2.5837733808 | 2.9847699259 | 0.8311249948 |
| H | 2.5874894707 | 2.9888934236 | -0.8222507612 |
| N | -2.4089108057 | 2.4125792878 | -0.0030658244 |
| H | -2.5839452371 | 2.9841553552 | -0.8320820915 |
| H | -2.5881194116 | 2.9895383621 | 0.821289367 |
| N | -2.4088373457 | -2.4125859825 | 0.0017422982 |
| H | -2.5850849873 | -2.9859628182 | 0.8292479003 |
| H | -2.5868292206 | -2.9877643924 | -0.8241336749 |

| | | | |
|---|--------------|---------------|---------------|
| N | 2.4090962111 | -2.4126095998 | -0.002684578 |
| H | 2.5847778829 | -2.9849075769 | -0.8310613201 |
| H | 2.5877528431 | -2.9888218597 | 0.8223174371 |

[(Al)Me₂(2,6-(NH₂)₂C₆H₃O)]₂ (5')

0,1

| | | | |
|----|---------------|---------------|---------------|
| C | -5.26467332 | 0.704980552 | 0.0018725279 |
| C | -4.8725714215 | -0.6301516156 | 0.0563821673 |
| C | -3.506235757 | -0.9631977471 | 0.0192060266 |
| C | -2.5658024182 | 0.0797992688 | -0.0643133703 |
| C | -2.9552799652 | 1.4290278317 | -0.1398502949 |
| C | -4.3276291483 | 1.7310518071 | -0.1010691677 |
| H | -6.3273065684 | 0.9520712319 | 0.0321175617 |
| H | -5.61586177 | -1.4272819221 | 0.1191059645 |
| H | -4.647459771 | 2.7738023083 | -0.1516852708 |
| O | -1.2033548755 | -0.2379038604 | -0.0560947509 |
| Al | 0.0614143337 | -0.4057024861 | -1.4470722377 |
| Al | -0.0613882821 | -0.4058026076 | 1.4470740196 |
| O | 1.203370044 | -0.2378222275 | 0.0561062558 |
| C | 2.5658020019 | 0.0799509073 | 0.0643442991 |
| C | 2.9552563696 | 1.42918838 | 0.1399540879 |
| C | 3.5062533004 | -0.9630184193 | -0.0192501107 |
| C | 4.327599756 | 1.731239669 | 0.1011767115 |
| C | 4.8725818066 | -0.6299447124 | -0.0564199289 |
| C | 5.264660606 | 0.7051912617 | -0.0018323921 |
| H | 4.647413364 | 2.7739938138 | 0.1518487144 |
| H | 5.6158851389 | -1.4270580487 | -0.1192025804 |
| H | 6.3272889433 | 0.9523033148 | -0.0320743345 |
| C | -0.1143312385 | 1.1393362289 | 2.658329026 |
| H | -0.575142547 | 2.0266139015 | 2.1955926589 |
| H | -0.7166155711 | 0.8972196221 | 3.548830208 |
| H | 0.8870720214 | 1.41827256 | 3.0250279997 |
| C | 0.1142431674 | 1.1395201479 | -2.6582235065 |
| H | 0.5749813201 | 2.0268017087 | -2.1954225614 |
| H | 0.71655117 | 0.8975101123 | -3.548737986 |
| H | -0.8871795936 | 1.4184033749 | -3.0249105821 |
| C | 0.1054457173 | -2.2553750088 | -2.1182062272 |
| C | -0.1052849395 | -2.2555244263 | 2.1180846533 |
| H | 1.0059297096 | -2.4535769982 | -2.7221972466 |
| H | 0.0647780979 | -3.0162568535 | -1.3212315234 |
| H | -0.7619088697 | -2.446303803 | -2.7710400898 |
| H | -0.0645644411 | -3.0163501407 | 1.3210585006 |
| H | 0.7620856262 | -2.4464360333 | 2.770902185 |
| H | -1.0057525662 | -2.4538318307 | 2.7220650992 |
| N | -3.0778107661 | -2.2866473421 | 0.0023045984 |
| H | -2.1163910493 | -2.4413130302 | 0.2931512834 |
| H | -3.7242014208 | -2.953709661 | 0.4114477734 |
| N | 1.9869534142 | 2.4368936857 | 0.1844447925 |

| | | | |
|---|---------------|---------------|---------------|
| H | 1.137574472 | 2.1853043766 | 0.6867572982 |
| H | 2.3485017381 | 3.3290112478 | 0.511459198 |
| N | 3.0778425022 | -2.2864744482 | -0.0024363641 |
| H | 2.1164197135 | -2.4411297754 | -0.2932813458 |
| H | 3.7242347001 | -2.9535012633 | -0.4116348615 |
| N | -1.9869800105 | 2.4367410519 | -0.1842738589 |
| H | -1.1375897784 | 2.1851833908 | -0.6865864797 |
| H | -2.3485279452 | 3.3288755058 | -0.511242539 |

[(Al)Me₂(2,6-(SH)₂C₆H₃O)]₂ (6)

0,1

| | | | |
|----|---------------|---------------|---------------|
| C | 5.4643420208 | 0.0004748946 | 0.0060016416 |
| C | 4.7537178853 | 1.1941927339 | 0.0868926536 |
| C | 3.3555224947 | 1.2061408289 | 0.1024007391 |
| C | 2.60721885 | 0.0004638502 | 0.0005391782 |
| C | 3.3559387591 | -1.2051525439 | -0.0990384089 |
| C | 4.7540450088 | -1.1932366397 | -0.07803437 |
| H | 6.5544095393 | 0.0004787545 | 0.0081775188 |
| H | 5.2779104686 | 2.1488546668 | 0.1485039544 |
| H | 5.2784570628 | -2.1478795779 | -0.1379972664 |
| O | 1.2634241504 | 0.0002751933 | -0.0016149353 |
| Al | -0.0004206477 | 1.515418152 | -0.0012385851 |
| Al | 0.0003378611 | -1.5155713409 | -0.0014784381 |
| O | -1.2635035898 | -0.0004712429 | -0.0019000316 |
| C | -2.6072957639 | -0.0006170897 | 0.0003976972 |
| C | -3.3560359534 | 1.2050058048 | -0.0989821294 |
| C | -3.3555676095 | -1.2063109349 | 0.1021745744 |
| C | -4.754138503 | 1.1930779265 | -0.0777695986 |
| C | -4.7537667901 | -1.1943725814 | 0.0868931144 |
| C | -5.4644125786 | -0.0006490248 | 0.006277163 |
| H | -5.2785681451 | 2.1477202933 | -0.1375839956 |
| H | -5.2779412722 | -2.1490488452 | 0.1484390126 |
| H | -6.5544797366 | -0.0006610574 | 0.0086325341 |
| C | -0.1502681333 | -2.0685391203 | -1.9042057055 |
| H | 0.6175545335 | -1.560497143 | -2.5116379 |
| H | -0.0317195828 | -3.1534032652 | -2.0549913252 |
| H | -1.1275108932 | -1.7895238412 | -2.3321359173 |
| C | 0.1505534501 | 2.0685109605 | -1.9039133192 |
| H | -0.6171617874 | 1.5604898366 | -2.5114991297 |
| H | 0.0320258437 | 3.1533795487 | -2.0546831645 |
| H | 1.1278713934 | 1.7895140574 | -2.3316885068 |
| C | -0.1518021743 | 2.0672541944 | 1.9018000683 |
| C | 0.151295895 | -2.067889811 | 1.9014382626 |
| H | -1.1287371642 | 1.786884408 | 2.3295758346 |
| H | 0.6165803514 | 1.5598958366 | 2.5090917876 |
| H | -0.0345809501 | 3.1521999974 | 2.0530500334 |
| H | -0.6171832562 | -1.5606716055 | 2.5087244655 |

| | | | |
|---|---------------|---------------|---------------|
| H | 0.0340025444 | -3.1528723863 | 2.0523681249 |
| H | 1.1281611102 | -1.7876774788 | 2.3294719823 |
| S | 2.5369879455 | -2.7883980822 | -0.2007920116 |
| H | 2.5418682275 | -2.893786889 | -1.5538480353 |
| S | 2.5362060321 | 2.7894874296 | 0.1997800564 |
| H | 2.5385679143 | 2.8973462316 | 1.5526443329 |
| S | -2.5371297421 | 2.7882669981 | -0.2008565335 |
| H | -2.5416492596 | 2.8933535068 | -1.5539389432 |
| S | -2.5361679463 | -2.7896433181 | 0.199102603 |
| H | -2.5384688626 | -2.8978682855 | 1.5519369175 |

[(Al)Me₂(2,6-(SH)₂C₆H₃O)]₂ (6')

0,1

| | | | |
|----|---------------|----------------|---------------|
| C | -5.3244730538 | -0.6713228932 | -0.0585063876 |
| C | -4.3960653137 | -1.7011155728 | 0.0620416549 |
| C | -3.0235990262 | -1.4175204854 | 0.1182904139 |
| C | -2.5804183166 | -0.0789882335 | 0.0484175597 |
| C | -3.5297886965 | 0.9622836445 | -0.0308881476 |
| C | -4.8981314237 | 0.6512609775 | -0.0889289872 |
| H | -6.3900965095 | -0.90005518754 | -0.101300597 |
| H | -4.7232584141 | -2.7394188903 | 0.1290423052 |
| H | -5.6234463378 | 1.4643311999 | -0.1492115173 |
| O | -1.2199715594 | 0.2104160614 | 0.0459594025 |
| Al | -0.0539556165 | 0.4073102751 | -1.4627990522 |
| Al | 0.054020417 | 0.4074840259 | 1.4626727079 |
| O | 1.2200306332 | 0.2103770716 | -0.0460650435 |
| C | 2.5804743757 | -0.0790401025 | -0.0484730055 |
| C | 3.5298450598 | 0.9622361776 | 0.0307476965 |
| C | 3.0236507335 | -1.4175822423 | -0.1181839641 |
| C | 4.8981836292 | 0.6512136351 | 0.0888791553 |
| C | 4.3961136703 | -1.7011775811 | -0.0618505319 |
| C | 5.3245214346 | -0.6713753325 | 0.0586217144 |
| H | 5.6234985596 | 1.4642873571 | 0.149107883 |
| H | 4.7233033532 | -2.7394908545 | -0.1287162208 |
| H | 6.3901418716 | -0.9006046418 | 0.1014901663 |
| C | 0.0098007162 | 2.2518646329 | 2.148021505 |
| H | 0.0082550455 | 3.0536711127 | 1.3938185186 |
| H | -0.8799875113 | 2.4018857592 | 2.7820708151 |
| H | 0.8897045114 | 2.4298289256 | 2.7877739039 |
| C | -0.0096612536 | 2.2516137279 | -2.148359723 |
| H | -0.0081060076 | 3.053506421 | -1.3942476827 |
| H | 0.880146036 | 2.4015362353 | -2.7824060453 |
| H | -0.8895437704 | 2.4295366203 | -2.7881524984 |
| C | -0.1492320237 | -1.0510283704 | -2.7763576814 |
| C | 0.1492106122 | -1.0507273415 | 2.7763787939 |
| H | 0.842360121 | -1.3157774456 | -3.178236008 |
| H | -0.6282625395 | -1.9754407014 | -2.4220975073 |
| H | -0.7423128628 | -0.6905409563 | -3.6338583415 |

| | | | |
|---|---------------|---------------|---------------|
| H | 0.6283937508 | -1.9751148904 | 2.4222584967 |
| H | 0.7421014916 | -0.6901196624 | 3.6339594035 |
| H | -0.8424229304 | -1.3155586769 | 3.1781002924 |
| S | -3.117599793 | 2.6775594823 | -0.0976014718 |
| H | -1.8060156985 | 2.5428712666 | 0.1966840628 |
| S | -1.9414967364 | -2.8174278141 | 0.1990374408 |
| H | -0.938734249 | -2.2374366876 | 0.9006865268 |
| S | 3.1176513793 | 2.6775165451 | 0.0973262676 |
| H | 1.8060657363 | 2.5428068757 | -0.1969463774 |
| S | 1.9415376488 | -2.817491936 | -0.1987656948 |
| H | 0.9388048572 | -2.2375768426 | -0.9005202003 |

[(Al)Me₂(2,6-(F)₂C₆H₃O)]₂ (7)

0,1

| | | | |
|----|---------------|---------------|---------------|
| C | -5.4227703674 | -0.0001146556 | -0.0004110098 |
| C | -4.7247388920 | -1.2096420501 | -0.0004006205 |
| C | -3.3366014272 | -1.1873783663 | -0.0002290154 |
| C | -2.5853882877 | -0.0000446315 | -0.0000612660 |
| C | -3.3366587418 | 1.1872540497 | -0.0000681047 |
| C | -4.7247981529 | 1.2094464126 | -0.0002430521 |
| H | -6.5088522998 | -0.0001410121 | -0.0005433397 |
| H | -5.2333474559 | -2.1691742114 | -0.0005194336 |
| H | -5.2334546668 | 2.1689533250 | -0.0002383665 |
| O | -1.2276614557 | -0.0000194144 | 0.0001199750 |
| Al | 0.0000097878 | -1.5019011793 | 0.0002369769 |
| Al | -0.0000112247 | 1.5018988151 | 0.0001169770 |
| O | 1.2276601761 | 0.0000176522 | 0.0004636633 |
| C | 2.5853870727 | 0.0000440776 | 0.0001962497 |
| C | 3.3366612561 | -1.1872525813 | 0.0001798420 |
| C | 3.3365966878 | 1.1873797735 | -0.0000423882 |
| C | 4.7248006927 | -1.2094410000 | -0.0001000700 |
| C | 4.7247341119 | 1.2096473638 | -0.0003019296 |
| C | 5.4227692840 | 0.0001220797 | -0.0003404063 |
| H | 5.2334600473 | -2.1689464276 | -0.0001187101 |
| H | 5.2333397157 | 2.1691810668 | -0.0004678003 |
| H | 6.5088512022 | 0.0001515947 | -0.0005541161 |
| C | 0.0000142360 | 2.3271886359 | -1.7902397203 |
| H | -0.8845594052 | 2.0336253042 | -2.3755586185 |
| H | 0.0008120997 | 3.4264405707 | -1.7417076546 |
| H | 0.8838019267 | 2.0323766362 | -2.3761207330 |
| C | 0.0004063018 | -2.3273303665 | -1.7900550068 |
| H | 0.8846843368 | -2.0331213869 | -2.3754992323 |
| H | 0.0004792624 | -3.4265789135 | -1.7414383079 |
| H | -0.8836775045 | -2.0332538494 | -2.3758565921 |
| C | -0.0003103992 | -2.3275099103 | 1.7904432446 |
| C | -0.0001139933 | 2.3276488239 | 1.7902574755 |
| H | 0.8838314671 | -2.0335299669 | 2.3762044380 |
| H | -0.8845329985 | -2.0333217003 | 2.3759813985 |

| | | | |
|---|---------------|---------------|---------------|
| H | -0.0004345864 | -3.4267534512 | 1.7417139155 |
| H | 0.8844353453 | 2.0342474452 | 2.3756943895 |
| H | -0.0009248409 | 3.4268883550 | 1.7414423229 |
| H | -0.8839286934 | 2.0329738257 | 2.3761662126 |
| F | 2.6593201212 | 2.3660746692 | 0.0000642632 |
| F | -2.6594510512 | 2.3659855100 | 0.0001096682 |
| F | -2.6593285386 | -2.3660754152 | -0.0001894525 |
| F | 2.6594578519 | -2.3659864970 | 0.0003909343 |

[(Al)Me₂(2,6-(F)₂C₆H₃O)]₂ (7')

0,1

| | | | |
|----|---------------|---------------|---------------|
| C | -5.3852700965 | -0.0000153308 | 0.0000014791 |
| C | -4.6942489041 | 1.2128374464 | 0.0000820736 |
| C | -3.3045221619 | 1.1950219118 | 0.000087865 |
| C | -2.5686398835 | -0.0000002607 | 0.0000021264 |
| C | -3.3045096255 | -1.1950304158 | -0.0000838131 |
| C | -4.6942363654 | -1.2128609322 | -0.0000785685 |
| H | -6.4753749723 | -0.0000207847 | 0.0000011905 |
| H | -5.2105164896 | 2.172491937 | 0.0001460389 |
| H | -5.2104940259 | -2.1725207763 | -0.0001429627 |
| O | -1.2023348221 | 0.0000006975 | 0.0000017258 |
| Al | 0.0000017569 | -0.000191772 | 1.4816311305 |
| Al | -0.0000023955 | 0.0002482849 | -1.4816304508 |
| O | 1.202333691 | 0.0000345307 | -0.0000010804 |
| C | 2.5686387505 | -0.000000955 | -0.0000017175 |
| C | 3.3045401264 | 1.1950096592 | 0.0002092595 |
| C | 3.3044891746 | -1.1950427347 | -0.000212792 |
| C | 4.6942673905 | 1.2128035197 | 0.000228667 |
| C | 4.6942154188 | -1.2128948647 | -0.0002322218 |
| C | 5.3852688341 | -0.0000604867 | -0.000001757 |
| H | 5.2105505 | 2.1724496589 | 0.0004204018 |
| H | 5.2104576475 | -2.1725629791 | -0.0004236737 |
| H | 6.4753737099 | -0.0000841779 | -0.000001711 |
| C | -0.0001591319 | -1.7366157308 | -2.3943741416 |
| H | -0.8829561545 | -2.3346067065 | -2.1180761018 |
| H | 0.0011739618 | -1.6316722863 | -3.4898583714 |
| H | 0.8810780075 | -2.3359332099 | -2.1160028995 |
| C | 0.0000468339 | -1.7373220409 | 2.3938676158 |
| H | 0.8820629601 | -2.3358785078 | 2.1163209221 |
| H | 0.0000756123 | -1.63271058 | 3.4893840359 |
| H | -0.881973931 | -2.3358957536 | 2.1163706714 |
| C | -0.0000329403 | 1.736690542 | 2.3943401684 |
| C | 0.0001489743 | 1.7373967613 | -2.3938323668 |
| H | 0.8820768505 | 2.335273627 | 2.1171404095 |
| H | -0.8819596065 | 2.3354035234 | 2.1168436002 |
| H | -0.0002197331 | 1.6317702826 | 3.4898273996 |
| H | 0.882908326 | 2.3353238825 | -2.1172812321 |
| H | -0.001115825 | 1.6328094321 | -3.4893503465 |

| | | | |
|---|---------------|---------------|---------------|
| H | -0.8811276902 | 2.3365861062 | -2.1153144607 |
| F | 2.6205410702 | -2.3601632969 | -0.0004830281 |
| F | -2.6205760541 | -2.3601572661 | -0.0001651269 |
| F | -2.6206047327 | 2.3601607036 | 0.0001686647 |
| F | 2.6206369449 | 2.3601543426 | 0.0004803779 |

[(B)Me₂(2,6-(OMe)₂C₆H₃O)]₂ (9)

0,1

| | | | |
|---|---------------|----------------|---------------|
| C | 4.9903436277 | 0.0388987043 | 0.8849305922 |
| C | 4.3782003122 | -1.1727551625 | 0.5798201718 |
| C | 3.1069123426 | -1.1905392445 | -0.0130266801 |
| C | 2.403509132 | 0.016274559 | -0.2481411115 |
| C | 3.0899259051 | 1.2346383105 | -0.0227492969 |
| C | 4.3613228524 | 1.2393598049 | 0.5701464136 |
| H | 5.9741442809 | 0.0476421148 | 1.3477428345 |
| H | 4.8894337912 | -2.1072260694 | 0.7828888768 |
| H | 4.8594312751 | 2.1824992371 | 0.7656289141 |
| O | 1.1100828504 | 0.0051399395 | -0.7455906806 |
| O | 2.4966026906 | -2.3388138153 | -0.4133182132 |
| O | 2.4638360024 | 2.3710838583 | -0.4323727092 |
| C | 2.934133141 | 3.6266805796 | 0.0466478069 |
| H | 2.2092325626 | 4.3646185011 | -0.30841133 |
| H | 2.976551178 | 3.6369138433 | 1.1458853306 |
| H | 3.9295848406 | 3.860457346 | -0.3601147095 |
| C | 2.9852964201 | -3.5839712024 | 0.0743929008 |
| H | 3.0283474206 | -3.5857404699 | 1.1736586994 |
| H | 2.2710297891 | -4.3348673704 | -0.2749965756 |
| H | 3.9838679667 | -3.8061557458 | -0.3312176443 |
| O | -1.1090476499 | -0.0102644022 | -0.7382043561 |
| C | -2.3990629624 | -0.0171640318 | -0.2318162225 |
| C | -3.083920836 | -1.2335848828 | 0.0084321871 |
| C | -3.1008617534 | 1.1915894608 | -0.0019875367 |
| C | -4.3512559266 | -1.2333004616 | 0.609982474 |
| C | -4.3681022082 | 1.1788096489 | 0.5996144871 |
| C | -4.9781432721 | -0.0302149966 | 0.918976182 |
| H | -4.8479954214 | -2.1747369016 | 0.8168064676 |
| H | -4.8779417202 | 2.1149696846 | 0.7983588 |
| H | -5.9587686562 | -0.03504500341 | 1.3885358055 |
| O | -2.4604940822 | -2.3734224893 | -0.395752506 |
| O | -2.493298009 | 2.3364799977 | -0.4159049348 |
| C | -2.9283398656 | -3.625085691 | 0.0957295584 |
| H | -2.2060680092 | -4.3660665546 | -0.2583433687 |
| H | -2.9637704283 | -3.6270051241 | 1.195267259 |
| H | -3.9264811883 | -3.8613987951 | -0.3028973271 |
| C | -2.9787573224 | 3.5856780136 | 0.0646128474 |
| H | -3.9800399263 | 3.8044819736 | -0.3361289971 |
| H | -3.0144347715 | 3.5966804873 | 1.1640914168 |
| H | -2.2668828863 | 4.3361011258 | -0.2958444173 |

| | | | |
|---|---------------|---------------|---------------|
| C | -0.0057783795 | 1.7243551712 | 0.9628835091 |
| H | 0.877410278 | 1.3804757765 | 1.5179727374 |
| H | -0.0135484455 | 2.8211782113 | 1.0037903688 |
| H | -0.8801176588 | 1.3678243127 | 1.5239824959 |
| C | 0.0183268079 | -1.7150470317 | 0.9772984019 |
| H | -0.8608680653 | -1.3660243611 | 1.53550962 |
| H | 0.0258469399 | -2.8114917912 | 1.0273945985 |
| H | 0.8966719205 | -1.3542610637 | 1.5293430775 |
| B | -0.0072006869 | 1.1914410071 | -0.5594278262 |
| B | 0.0095535596 | -1.1949939852 | -0.5494268686 |
| C | -0.0180054258 | 2.1354981528 | -1.8598062207 |
| C | 0.0117033025 | -2.1499993142 | -1.8418305671 |
| H | 0.8668957964 | 1.9613522715 | -2.4848628908 |
| H | -0.9044268057 | 1.94893726 | -2.4791090843 |
| H | -0.0245852602 | 3.2007244475 | -1.5911036568 |
| H | 0.0214781981 | -3.2129087639 | -1.5641694011 |
| H | -0.8780474191 | -1.982055253 | -2.4616667169 |
| H | 0.8932620279 | -1.9677992323 | -2.4693231948 |

[(B)Me₂(2,6-(OMe)₂C₆H₃O)]₂ (9')

0,1

| | | | |
|---|---------------|---------------|---------------|
| C | -5.218106953 | 0.0725959144 | 0.0666470898 |
| C | -4.5428250931 | -0.0108961632 | -1.1503911537 |
| C | -3.1376900774 | -0.0190356286 | -1.1613592894 |
| C | -2.4298549138 | 0.0570976421 | 0.054874224 |
| C | -3.1265307132 | 0.141006317 | 1.2770672322 |
| C | -4.5316793753 | 0.1485066847 | 1.2779700267 |
| H | -6.3058913279 | 0.078649802 | 0.0712498244 |
| H | -5.1015299348 | -0.0689252201 | -2.0797991015 |
| H | -5.0818819153 | 0.2126436635 | 2.2102468011 |
| O | -1.0574018632 | 0.0493787554 | 0.0491179497 |
| O | -2.3782843078 | -0.0969045651 | -2.2859007228 |
| O | -2.3568202871 | 0.2102083315 | 2.3951450382 |
| C | -3.0146112096 | 0.2972339026 | 3.6562596885 |
| H | -2.2161214435 | 0.3421260616 | 4.4021053806 |
| H | -3.6352119093 | 1.2040801491 | 3.7178165609 |
| H | -3.6451106019 | -0.5867225974 | 3.8362667274 |
| C | -3.0476511933 | -0.1759684172 | -3.5414494032 |
| H | -3.6695759888 | 0.7151552253 | -3.7158365928 |
| H | -2.2560491738 | -0.2296246388 | -4.2940257245 |
| H | -3.6789812056 | -1.0757017036 | -3.5980447741 |
| O | 1.0572499824 | 0.0372647023 | 0.0407304126 |
| C | 2.4297161936 | 0.0292482389 | 0.0353715254 |
| C | 3.126741196 | -0.0553839162 | -1.1865351186 |
| C | 3.1371798389 | 0.1057793115 | 1.2518256092 |
| C | 4.5319100599 | -0.063346211 | -1.1869795704 |
| C | 4.5422973732 | 0.097172072 | 1.2413107078 |

| | | | |
|---|---------------|---------------|---------------|
| C | 5.2179571431 | 0.0128926443 | 0.0245133529 |
| H | 5.0823644707 | -0.1280620292 | -2.1190663873 |
| H | 5.1007320654 | 0.1554572426 | 2.1690686854 |
| H | 6.3057410543 | 0.0064763031 | 0.0203019907 |
| O | 2.3573725428 | -0.1249498387 | -2.3048385177 |
| O | 2.3774497776 | 0.1845544496 | 2.3760475502 |
| C | 3.015582007 | -0.2112674406 | -3.5657993659 |
| H | 2.2173353971 | -0.2557638758 | -4.3119271274 |
| H | 3.6461278699 | 0.6727991631 | -3.7450673337 |
| H | 3.6361918179 | -1.1180837941 | -3.6276855837 |
| C | 3.0464050035 | 0.2630566387 | 3.6318391943 |
| H | 3.6678868711 | -0.6283707537 | 3.8062529412 |
| H | 3.6781146011 | 1.1625016426 | 3.6888514008 |
| H | 2.2545626289 | 0.3168961154 | 4.3841510273 |
| C | -0.0046057516 | -1.8856160056 | 1.5467259866 |
| H | -0.8904114859 | -2.5317933525 | 1.6474507517 |
| H | 0.8757081251 | -2.5404668377 | 1.6397978876 |
| H | 0.0025961267 | -1.1802368133 | 2.3841216460 |
| C | 0.0167626108 | 2.1526099175 | 1.2806988370 |
| H | 0.0170841107 | 1.5632745614 | 2.2034710661 |
| H | 0.9035827056 | 2.8052245480 | 1.2877875922 |
| H | -0.8624924257 | 2.8152690343 | 1.2947535752 |
| B | -0.0065207888 | -1.1558976234 | 0.1236856589 |
| B | 0.0063683079 | 1.2425824597 | -0.0342673888 |
| C | -0.0172802260 | -2.0654291538 | -1.1916345200 |
| C | 0.0050615086 | 1.9717576594 | -1.4575692247 |
| H | -0.9041323093 | -2.7179917860 | -1.1987670221 |
| H | -0.0178152432 | -1.4756662031 | -2.1141396342 |
| H | 0.8619814866 | -2.7280604209 | -1.2062448005 |
| H | -0.8746283166 | 2.6273050008 | -1.5513002686 |
| H | 0.8914884409 | 2.6171642548 | -1.5580598832 |
| H | -0.0022075220 | 1.2660631403 | -2.2946955038 |

[(Ga)Me₂(2,6-(OMe)₂C₆H₃O)]₂ (10)

0,1

| | | | |
|---|--------------|---------------|---------------|
| C | 5.1837689627 | -0.0069340056 | 0.9885363790 |
| C | 4.5430896853 | -1.2182083050 | 0.7219135667 |
| C | 3.2471948648 | -1.2124958209 | 0.1945420693 |
| C | 2.5589525756 | -0.0033914557 | -0.0495054271 |
| C | 3.2506857839 | 1.2038757246 | 0.1938898920 |
| C | 4.5465827934 | 1.2060543835 | 0.7212988208 |
| H | 6.1898095085 | -0.0082764156 | 1.4001074356 |
| H | 5.0501611395 | -2.1577550356 | 0.9162146627 |
| H | 5.0563808883 | 2.1442136500 | 0.9151673915 |
| O | 1.2889678741 | -0.0017117232 | -0.5102159664 |
| O | 2.5410263250 | -2.3452512911 | -0.1336731634 |
| O | 2.5478273662 | 2.3384789159 | -0.1348834877 |
| C | 3.0206409711 | 3.5925130759 | 0.3506222704 |

| | | | |
|----|---------------|---------------|---------------|
| H | 2.2618444818 | 4.3271477405 | 0.0665612491 |
| H | 3.1354791677 | 3.5698660346 | 1.4441281593 |
| H | 3.9822267395 | 3.8549507875 | -0.1141388844 |
| C | 3.0097454451 | -3.6003130860 | 0.3532083673 |
| H | 3.1245999256 | -3.5768599032 | 1.4466882932 |
| H | 2.2485874122 | -4.3327936602 | 0.0699059178 |
| H | 3.9704892545 | -3.8663467798 | -0.1112400520 |
| O | -1.2936289215 | 0.0015833071 | -0.5216784141 |
| C | -2.5621968951 | 0.0032232708 | -0.0555406728 |
| C | -3.2532375952 | -1.2039141731 | 0.1913426159 |
| C | -3.2497619149 | 1.2121631159 | 0.1921304504 |
| C | -4.5452739061 | -1.2061168057 | 0.7280865457 |
| C | -4.5417914336 | 1.2178086918 | 0.7288446321 |
| C | -5.1804381709 | 0.0066780647 | 1.0005977367 |
| H | -5.0535603651 | -2.1444073070 | 0.9253007239 |
| H | -5.0473619911 | 2.1574479892 | 0.9266158748 |
| H | -6.1833021450 | 0.0079860868 | 1.4198561740 |
| O | -2.5542959643 | -2.3389156867 | -0.1442886791 |
| O | -2.5475053417 | 2.3453634441 | -0.1428132701 |
| C | -3.0197991844 | -3.5926567823 | 0.3496222414 |
| H | -2.2638883168 | -4.3269656235 | 0.0569137071 |
| H | -3.1204857667 | -3.5679030689 | 1.4444307640 |
| H | -3.9869954631 | -3.8568734449 | -0.1022455865 |
| C | -3.0090968242 | 3.6001012086 | 0.3522836436 |
| H | -3.9754889493 | 3.8677061561 | -0.0993016495 |
| H | -3.1097957309 | 3.5746473325 | 1.4470694182 |
| H | -2.2509397621 | 4.3323441683 | 0.0602102935 |
| C | -0.0070009966 | 1.9583717240 | 1.6787457745 |
| H | 0.8820685607 | 1.5105515825 | 2.1417408039 |
| H | -0.0092070316 | 3.0323527506 | 1.9122835588 |
| H | -0.8971374814 | 1.5079068744 | 2.1370925452 |
| C | -0.0131472222 | -1.9587198369 | 1.6785710909 |
| H | -0.9027908041 | -1.5065741835 | 2.1362085366 |
| H | -0.0176262671 | -3.0327155465 | 1.9120020843 |
| H | 0.8763960702 | -1.5126639878 | 2.1423684542 |
| C | 0.0091790471 | -2.5998156073 | -2.0175046649 |
| C | 0.0157048661 | 2.5998677310 | -2.0172250218 |
| H | -0.9530956278 | -2.4806951354 | -2.5302530294 |
| H | 0.8072241861 | -2.2078470943 | -2.6605390400 |
| H | 0.1901138667 | -3.6744407420 | -1.8711725467 |
| H | -0.9469618702 | 2.4837870282 | -2.5299408505 |
| H | 0.1999275663 | 3.6739079001 | -1.8707077584 |
| H | 0.8125081520 | 2.2055738373 | -2.6603728299 |
| Ga | -0.0003247215 | 1.6123152456 | -0.2897716581 |
| Ga | -0.0040818154 | -1.6124703144 | -0.2899024917 |

[(Ga)Me₂(2,6-(OMe)₂C₆H₃O)]₂ (10')

0,1

| | | | |
|---|---------------|---------------|---------------|
| C | 5.4133554826 | -0.000043376 | 0.0001777284 |
| C | 4.7289259327 | 0.0000698328 | -1.2157807164 |
| C | 3.3251929855 | 0.0000891452 | -1.2177483002 |
| C | 2.6107883537 | 0.0000025194 | 0.0000350046 |
| C | 3.3250695683 | -0.0001071255 | 1.2178889641 |
| C | 4.72880165 | -0.0001339175 | 1.2160661992 |
| H | 6.5009484905 | -0.0000607575 | 0.0002333909 |
| H | 5.2825589904 | 0.0001454023 | -2.1486658218 |
| H | 5.2823374994 | -0.0002260578 | 2.1490091743 |
| O | 1.2486062754 | 0.0000265358 | -0.0000240035 |
| O | 2.5523050997 | 0.0002224235 | -2.3455820042 |
| O | 2.5520609994 | -0.0002100220 | 2.3456375857 |
| C | 3.2174783362 | -0.0003428132 | 3.6059793651 |
| H | 2.4246817861 | -0.0004073800 | 4.3595226427 |
| H | 3.8450292513 | -0.8970937471 | 3.7232278069 |
| H | 3.8450498054 | 0.8963708075 | 3.7234029888 |
| C | 3.2178591641 | 0.0003384942 | -3.6058528916 |
| H | 3.8454135071 | -0.8963953249 | -3.7232124062 |
| H | 2.4251445085 | 0.0004321611 | -4.3594824858 |
| H | 3.8454519178 | 0.8970692655 | -3.7230303587 |
| O | -1.2486054709 | 0.0000712988 | 0.0000296296 |
| C | -2.6107875329 | 0.0000967075 | 0.0000373889 |
| C | -3.3251170511 | -0.0000056668 | 1.2178623558 |
| C | -3.3251435815 | 0.0002223857 | -1.2177749594 |
| C | -4.7288494529 | 0.0000007266 | 1.2159812550 |
| C | -4.7288762194 | 0.0002635651 | -1.2158657458 |
| C | -5.4133544916 | 0.0001439731 | 0.0000650674 |
| H | -5.2824241592 | -0.0001109900 | 2.1489010512 |
| H | -5.2824704202 | 0.0003906003 | -2.1487740387 |
| H | -6.5009475015 | 0.0001611001 | 0.0000770495 |
| O | -2.5521561986 | -0.0002156669 | 2.3456454196 |
| O | -2.5522074549 | 0.0003945829 | -2.3455737132 |
| C | -3.2176324111 | -0.0004225651 | 3.6059566339 |
| H | -2.4248713591 | -0.0005684822 | 4.3595373905 |
| H | -3.8451802998 | 0.8963027939 | 3.7234159948 |
| H | -3.8452174860 | -0.8971618867 | 3.7231098371 |
| C | -3.2177020814 | 0.0005975032 | -3.6058754237 |
| H | -3.8452829316 | -0.8961082815 | -3.7233084827 |
| H | -3.8452577549 | 0.8973561138 | -3.7230393647 |
| H | -2.4249515980 | 0.0007002539 | -4.3594671631 |
| C | 0.0001786417 | 2.4161072938 | 1.8183442611 |
| H | 0.8888574919 | 2.0820853110 | 2.3684307211 |
| H | -0.0002311789 | 3.5134849279 | 1.7731909979 |
| H | -0.8879820240 | 2.0814282446 | 2.3688635261 |
| C | -0.0000411589 | -2.4161348299 | 1.8181655514 |
| H | -0.8884229179 | -2.0817561228 | 2.3685174136 |
| H | -0.0001260258 | -3.5135088894 | 1.7729335219 |

| | | | |
|----|---------------|---------------|---------------|
| H | 0.8884177168 | -2.0818906913 | 2.3684710982 |
| C | -0.0000538739 | -2.4159875703 | -1.8183509192 |
| C | -0.0000878155 | 2.4162141999 | -1.8181710053 |
| H | -0.8885437014 | -2.0817271924 | -2.3685934977 |
| H | 0.8882957378 | -2.0815297386 | -2.3687022661 |
| H | 0.0000699626 | -3.5133660790 | -1.7732155330 |
| H | -0.8887650425 | 2.0822358074 | -2.3682879620 |
| H | 0.0003363971 | 3.5135889189 | -1.7729542172 |
| H | 0.8880751233 | 2.0815555371 | -2.3687010534 |
| Ga | 0.0000296558 | 1.5905741970 | 0.0000629871 |
| Ga | -0.0000296652 | -1.5904760306 | -0.0000588990 |

[(In)Me₂(2,6-(OMe)₂C₆H₃O)]₂ (11)

0,1

| | | | |
|---|---------------|---------------|---------------|
| C | -5.1803115520 | -0.0003990209 | -0.8956503816 |
| C | -4.5588090809 | -1.2119848898 | -0.5872798516 |
| C | -3.3069509807 | -1.2077391806 | 0.0351745697 |
| C | -2.6318444263 | -0.0017993996 | 0.3459384004 |
| C | -3.3119357128 | 1.2045974310 | 0.0482040899 |
| C | -4.5636426338 | 1.2102754912 | -0.5747174970 |
| H | -6.1523269009 | 0.0001754343 | -1.3818935036 |
| H | -5.0495853006 | -2.1499190881 | -0.8266951729 |
| H | -5.0580778377 | 2.1487908047 | -0.8041844428 |
| O | -1.4133766006 | -0.0023911532 | 0.9025590928 |
| O | -2.6295845956 | -2.3518034922 | 0.4048537110 |
| O | -2.6404830678 | 2.3478175633 | 0.4316206344 |
| C | -3.0971117272 | 3.6015985387 | -0.0702518710 |
| H | -2.3743098829 | 4.3444765208 | 0.2804010919 |
| H | -3.1313139223 | 3.5941036994 | -1.1695382839 |
| H | -4.0942221414 | 3.8418198016 | 0.3260052959 |
| C | -3.0916565853 | -3.6043508013 | -0.0944964745 |
| H | -3.1373065904 | -3.5953470776 | -1.1933489205 |
| H | -2.3654656675 | -4.3478771165 | 0.2475857206 |
| H | -4.0848660650 | -3.8445452181 | 0.3115445478 |
| O | 1.4172164361 | 0.0017626147 | 0.9059354620 |
| C | 2.6350461721 | 0.0017259957 | 0.3476073871 |
| C | 3.3150026398 | -1.204340052 | 0.0474205754 |
| C | 3.3099129853 | 1.2078651303 | 0.0364396561 |
| C | 4.5641300486 | -1.2094041608 | -0.5806547590 |
| C | 4.5592276334 | 1.2125503676 | -0.5911334591 |
| C | 5.1794193861 | 0.0013954774 | -0.9035020736 |
| H | 5.0577713850 | -2.1477376998 | -0.8125445750 |
| H | 5.0491735831 | 2.1506973952 | -0.8313813949 |
| H | 6.1491817292 | 0.0012494283 | -1.3942236149 |
| O | 2.6465231981 | -2.3483402037 | 0.4338610178 |
| O | 2.6355370727 | 2.3521477906 | 0.4111793364 |
| C | 3.0990015547 | -3.6009944061 | -0.0750631731 |
| H | 2.3787174277 | -4.3447745473 | 0.2789111599 |

| | | | |
|----|---------------|---------------|---------------|
| H | 3.1249966965 | -3.5902342984 | -1.1745345906 |
| H | 4.0990104314 | -3.8426996713 | 0.3129065225 |
| C | 3.0928098386 | 3.6041830235 | -0.0944202589 |
| H | 4.0888774275 | 3.8461387446 | 0.3034972128 |
| H | 3.1301866351 | 3.5926685754 | -1.1935354725 |
| H | 2.3687174009 | 4.3479991560 | 0.2514970387 |
| C | -0.0037575726 | 1.9226667868 | -1.5684894514 |
| H | -0.9350156615 | 1.4914906885 | -1.9526243333 |
| H | 0.0768258641 | 2.9627924814 | -1.9065953060 |
| H | 0.8471468416 | 1.3519350057 | -1.9565848266 |
| C | 0.0142148936 | -1.9211247410 | -1.5709889704 |
| H | 0.9490072661 | -1.4949404671 | -1.9520351638 |
| H | -0.0716066808 | -2.9605115236 | -1.9100616694 |
| H | -0.8322545765 | -1.3451960625 | -1.9611537138 |
| C | -0.0089000966 | -2.7982463185 | 2.5213038182 |
| C | -0.0048843108 | 2.7951088594 | 2.5252078693 |
| H | 0.9749441643 | -2.6896835341 | 2.9901861878 |
| H | -0.7751930133 | -2.3353842153 | 3.1529200869 |
| H | -0.2387819186 | -3.8643742540 | 2.4039536717 |
| H | 0.9834102254 | 2.6920871056 | 2.9859486963 |
| H | -0.2425779933 | 3.8599199250 | 2.4116053645 |
| H | -0.7629387110 | 2.3263561369 | 3.1624030520 |
| In | -0.0013324104 | 1.7833243319 | 0.6052980834 |
| In | 0.0044052797 | | |

[(In)Me₂(2,6-(OMe)₂C₆H₃O)]₂ (11')

0,1

| | | | |
|---|---------------|---------------|---------------|
| C | -5.5120420000 | 0.0007180000 | -0.0000160000 |
| C | -4.8257390000 | -1.2149550000 | -0.0002060000 |
| C | -3.4227330000 | -1.2158420000 | -0.0002050000 |
| C | -2.6999660000 | 0.0000570000 | -0.0000130000 |
| C | -3.4221690000 | 1.2162940000 | 0.0001790000 |
| C | -4.8251720000 | 1.2160700000 | 0.0001760000 |
| H | -6.5995730000 | 0.0009730000 | -0.0000160000 |
| H | -5.3796160000 | -2.1480080000 | -0.0003600000 |
| H | -5.3786100000 | 2.1493840000 | 0.0003310000 |
| O | -1.3505880000 | -0.0002520000 | -0.0000070000 |
| O | -2.6473780000 | -2.3468690000 | -0.0004140000 |
| O | -2.6462710000 | 2.3469420000 | 0.0003980000 |
| C | -3.3135340000 | 3.6052720000 | 0.0000604000 |
| H | -2.5229440000 | 4.3615320000 | 0.0007570000 |
| H | -3.9422220000 | 3.7224770000 | -0.8956980000 |
| H | -3.9422640000 | 3.7221630000 | 0.8969180000 |
| C | -3.3152740000 | -3.6048650000 | -0.0006060000 |
| H | -3.9440610000 | -3.7214470000 | -0.8969190000 |
| H | -2.5250690000 | -4.3615270000 | -0.0007470000 |
| H | -3.9440220000 | -3.7217380000 | 0.8956970000 |
| O | 1.3505870000 | 0.0001840000 | 0.0000110000 |

| | | | |
|----|---------------|---------------|---------------|
| C | 2.6999650000 | 0.0000700000 | 0.0000150000 |
| C | 3.4225660000 | 1.2160700000 | 0.0002270000 |
| C | 3.4223340000 | -1.2160660000 | -0.0001960000 |
| C | 4.8255700000 | 1.2153760000 | 0.0002170000 |
| C | 4.8253370000 | -1.2156490000 | -0.0001840000 |
| C | 5.5120400000 | -0.0002020000 | 0.0000170000 |
| H | 5.3793200000 | 2.1485060000 | 0.0003680000 |
| H | 5.3789040000 | -2.1488870000 | -0.0003330000 |
| H | 6.5995720000 | -0.0003060000 | 0.0000170000 |
| O | 2.6470610000 | 2.3469920000 | 0.0004080000 |
| O | 2.6465830000 | -2.3468180000 | -0.0003790000 |
| C | 3.3147980000 | 3.6050720000 | 0.0005350000 |
| H | 2.5244960000 | 4.3616340000 | 0.0006300000 |
| H | 3.9435660000 | 3.7217840000 | 0.8968450000 |
| H | 3.9435350000 | 3.7219790000 | -0.8957710000 |
| C | 3.3140040000 | -3.6050640000 | -0.0005900000 |
| H | 3.9427390000 | -3.7218740000 | -0.8969100000 |
| H | 3.9427160000 | -3.7221890000 | 0.8957060000 |
| H | 2.5235090000 | -4.3614240000 | -0.0007320000 |
| C | -0.0004860000 | 2.0716410000 | 2.4484900000 |
| H | -0.8965490000 | 2.5485190000 | 2.0372380000 |
| H | 0.0015810000 | 2.1461650000 | 3.5412360000 |
| H | 0.8932210000 | 2.5498950000 | 2.0337290000 |
| C | -0.0001830000 | 2.0731920000 | -2.4473140000 |
| H | 0.8946210000 | 2.5506230000 | -2.0339680000 |
| H | -0.0001010000 | 2.1483240000 | -3.5400200000 |
| H | -0.8951570000 | 2.5504140000 | -2.0341070000 |
| C | 0.0002310000 | -2.0719980000 | -2.4481520000 |
| C | 0.0004480000 | -2.0735470000 | 2.4469890000 |
| H | 0.8953950000 | -2.5492950000 | -2.0354360000 |
| H | -0.8943830000 | -2.5496870000 | -2.0346890000 |
| H | -0.0002110000 | -2.1467060000 | -3.5408870000 |
| H | 0.8964370000 | -2.5501540000 | 2.0352650000 |
| H | -0.0014720000 | -2.1488590000 | 3.5396820000 |
| H | -0.8933420000 | -2.5514510000 | 2.0320050000 |
| In | -0.0000130000 | -0.0007090000 | 1.7733740000 |
| In | 0.0000140000 | 0.0004610000 | -1.7733700000 |

[(Ti)Me₂(2,6-(OMe)₂C₆H₃O)]₂ (12)

0,1

| | | | |
|---|--------------|---------------|---------------|
| C | 5.3558913009 | -0.0072500277 | 1.1654133769 |
| C | 4.7248186863 | -1.2158071555 | 0.8636989758 |
| C | 3.4590581369 | -1.2103295435 | 0.2703074929 |
| C | 2.7604397567 | -0.0036117924 | -0.0251746445 |
| C | 3.4624482600 | 1.2011399076 | 0.2702872763 |
| C | 4.7282250657 | 1.2030730775 | 0.8636673972 |
| H | 6.3390449688 | -0.0086322176 | 1.6287229445 |
| H | 5.2246308909 | -2.1535512345 | 1.0857242028 |

| | | | |
|---|---------------|---------------|---------------|
| H | 5.2306772808 | 2.1394097027 | 1.0856743839 |
| O | 1.5479344912 | -0.0019116417 | -0.5566952554 |
| O | 2.7829071777 | -2.3656496531 | -0.0879091515 |
| O | 2.7895434953 | 2.3583574131 | -0.0879761086 |
| C | 3.3279124013 | 3.6041630826 | 0.3383743775 |
| H | 2.6146895559 | 4.3684728855 | 0.0122060010 |
| H | 3.4371467373 | 3.6349873814 | 1.4334505841 |
| H | 4.3070920866 | 3.7932950400 | -0.1267012597 |
| C | 3.3179321303 | -3.6129551188 | 0.3382618955 |
| H | 3.4271066440 | -3.6442250837 | 1.4333328696 |
| H | 2.6026650292 | -4.3753091949 | 0.0119963461 |
| H | 4.2965932165 | -3.8046436660 | -0.1268582883 |
| O | -1.5424257979 | 0.0019217466 | -0.5608515927 |
| C | -2.7568708241 | 0.0035676940 | -0.0343644437 |
| C | -3.4605848090 | -1.2010916030 | 0.2584183743 |
| C | -3.4570681863 | 1.2101294336 | 0.2589952387 |
| C | -4.7256106377 | -1.2030721477 | 0.8533076849 |
| C | -4.7220828950 | 1.2154950510 | 0.8538861016 |
| C | -5.3528417409 | 0.0070599092 | 1.1566427158 |
| H | -5.2281364890 | -2.1394811634 | 1.0748646726 |
| H | -5.2218793965 | 2.1532666395 | 1.0758676328 |
| H | -6.3349172169 | 0.0083885131 | 1.6222198217 |
| O | -2.7897803339 | -2.3585544540 | -0.1038697848 |
| O | -2.7829848763 | 2.3658424181 | -0.1027227499 |
| C | -3.3252892222 | -3.6042480659 | 0.3271449938 |
| H | -2.6143015698 | -4.3687360173 | -0.0034245688 |
| H | -3.4272485586 | -3.6340257222 | 1.4229494638 |
| H | -4.3075496071 | -3.7939108135 | -0.1311410962 |
| C | -3.3148909362 | 3.6127609593 | 0.3292022049 |
| H | -4.2966611558 | 3.8055268388 | -0.1288426902 |
| H | -3.4166426442 | 3.6420766257 | 1.4250370654 |
| H | -2.6017877327 | 4.3754760590 | -0.0009083601 |
| C | 0.0015066008 | 1.8892142935 | 1.8872872052 |
| H | 0.9006190271 | 1.3457930311 | 2.1907630596 |
| H | 0.0044917702 | 2.9009867157 | 2.3062177438 |
| H | -0.9019606897 | 1.3518110852 | 2.1885929868 |
| C | -0.0031809709 | -1.8883126544 | 1.8874597771 |
| H | -0.9046421875 | -1.3476344970 | 2.1889242628 |
| H | -0.0035787392 | -2.8999212337 | 2.3067940733 |
| H | 0.8979536887 | -1.3479017153 | 2.1903114444 |
| C | -0.0040312078 | -2.4350243230 | -2.4301728624 |
| C | 0.0015083495 | 2.4336204247 | -2.4306480628 |
| H | -1.0456442399 | -2.4904999780 | -2.7578146967 |
| H | 0.5186715559 | -1.6061902811 | -2.9150943661 |
| H | 0.5194429608 | -3.3787326099 | -2.6129454460 |
| H | -1.0399908753 | 2.5068961239 | -2.7551976257 |
| H | 0.5408786425 | 3.3678295152 | -2.6159216042 |
| H | 0.5080852124 | 1.5953608954 | -2.9164732282 |

| | | | |
|----|---------------|---------------|---------------|
| Tl | 0.0045789212 | 1.9510098099 | -0.3031451898 |
| Tl | -0.0009455009 | -1.9509636640 | -0.3029645711 |

[(Tl)Me₂(2,6-(OMe)₂C₆H₃O)]₂ (12')

0,1

| | | | |
|---|---------------|---------------|---------------|
| C | -5.6058336730 | 0.0005336206 | -0.0000108273 |
| C | -4.9148739023 | -1.2129988213 | 0.0001056122 |
| C | -3.5132086265 | -1.2124631342 | 0.0000400031 |
| C | -2.7724730821 | 0.0001829183 | -0.0000017416 |
| C | -3.5128982014 | 1.2130063236 | -0.0000461439 |
| C | -4.9145623096 | 1.2138903418 | -0.0001212040 |
| H | -6.6932683970 | 0.0006721511 | -0.0000142007 |
| H | -5.4688142434 | -2.1464405304 | 0.0002266159 |
| H | -5.4682647617 | 2.1474723600 | -0.0002442903 |
| O | -1.4389561847 | -0.0000046422 | 0.0000013459 |
| O | -2.7440718647 | -2.3558969982 | 0.0000193744 |
| O | -2.7434584406 | 2.3562350724 | -0.0000140208 |
| C | -3.4224405170 | 3.6061485681 | -0.0005859299 |
| H | -2.6406679724 | 4.3724127608 | -0.0005392966 |
| H | -4.0533354333 | 3.7182530365 | -0.8964772307 |
| H | -4.0539561736 | 3.7187763606 | 0.8948157249 |
| C | -3.4233838366 | -3.6056338719 | 0.0005738724 |
| H | -4.0549184472 | -3.7180896658 | -0.8948357690 |
| H | -2.6418152268 | -4.3721066081 | 0.0005286409 |
| H | -4.0543355550 | -3.7175826081 | 0.8964584902 |
| O | 1.4389506048 | -0.0000711293 | 0.0000003731 |
| C | 2.7724667081 | -0.0001302034 | 0.0000002524 |
| C | 3.5130706456 | 1.2125940366 | 0.0001567594 |
| C | 3.5130175579 | -1.2128771151 | -0.0001625047 |
| C | 4.9147354726 | 1.2132797545 | 0.0000892318 |
| C | 4.9146821624 | -1.2136112977 | -0.0000916468 |
| C | 5.6058236408 | -0.0001798253 | 0.0000012970 |
| H | 5.4685758979 | 2.1467810434 | 0.0001245180 |
| H | 5.4684852405 | -2.1471335665 | -0.0001308538 |
| H | 6.6932583874 | -0.0002021911 | 0.0000017985 |
| O | 2.7438059486 | 2.3559415523 | 0.0003703399 |
| O | 2.7436957612 | -2.3561854550 | -0.0003956613 |
| C | 3.4229847051 | 3.6057505514 | 0.0002023537 |
| H | 2.6413345474 | 4.3721400090 | 0.0004135198 |
| H | 4.0544549843 | 3.7180221420 | 0.8956801099 |
| H | 4.0539782628 | 3.7180171177 | -0.8956137347 |
| C | 3.4228049983 | -3.6060303872 | -0.0002196299 |
| H | 4.0542775475 | -3.7183377908 | -0.8956914252 |
| H | 4.0537861510 | -3.7183279977 | 0.8956014074 |
| H | 2.6411097786 | -4.3723733933 | -0.0004356666 |
| C | 0.0000040784 | 2.1778301280 | 2.2058212106 |
| H | -0.9028379779 | 2.5286528647 | 1.6998169844 |

| | | | |
|----|---------------|---------------|---------------|
| H | 0.0025738237 | 2.4473288979 | 3.2667213470 |
| H | 0.9002812211 | 2.5288796004 | 1.6954224830 |
| C | 0.0004451140 | 2.1806663661 | -2.2034975121 |
| H | 0.9027561961 | 2.5307022832 | -1.6960198951 |
| H | -0.0008797122 | 2.4513653531 | -3.2640866976 |
| H | -0.9003206814 | 2.5312037777 | -1.6936338608 |
| C | -0.0004026272 | -2.1779465734 | -2.2057480773 |
| C | 0.0000123582 | -2.1807827719 | 2.2034328815 |
| H | 0.9005838435 | -2.5290845479 | -1.6966658197 |
| H | -0.9025406773 | -2.5286430313 | -1.6984013252 |
| H | 0.0005458208 | -2.4474814630 | -3.2666420126 |
| H | 0.9028970618 | -2.5309372478 | 1.6970630607 |
| H | -0.0026903738 | -2.4515160429 | 3.2640110152 |
| H | -0.9001755927 | -2.5311671159 | 1.6924426693 |
| TI | 0.0000075528 | -0.0013252032 | 1.9384543030 |
| TI | 0.0000044132 | 0.0012172413 | -1.9384516172 |