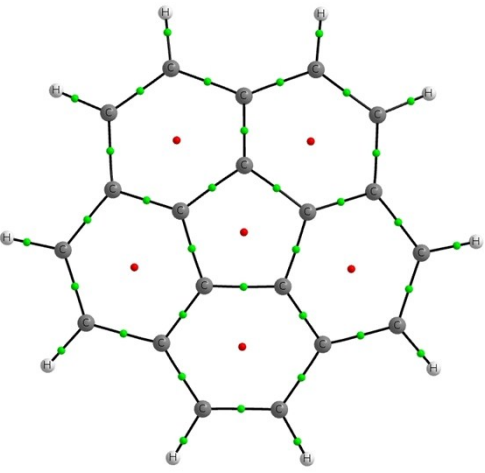
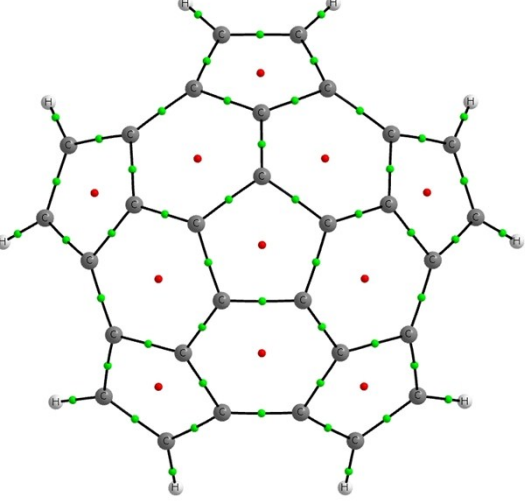
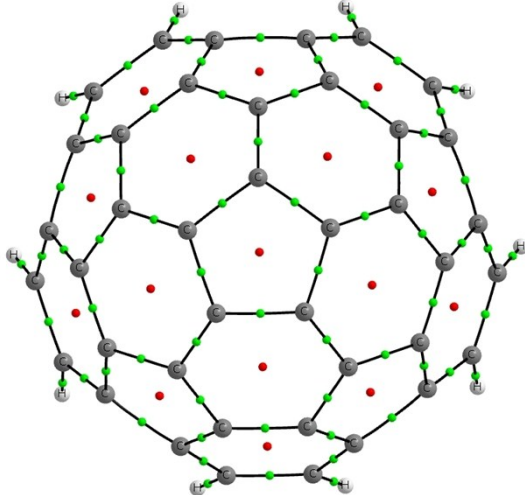
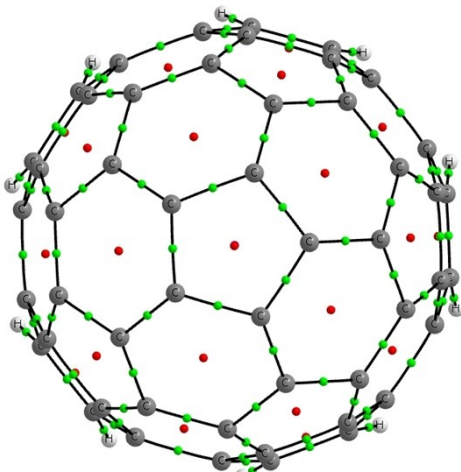
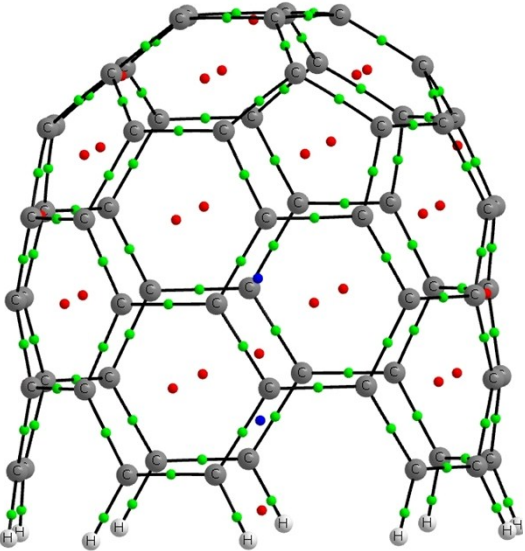


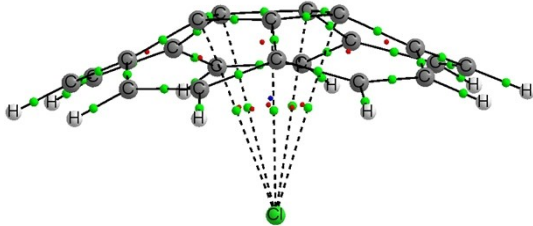
Table S1 Molecular Graph; M06-2X/6-311+G(d) energy(au), Cartesian coordinates (Å) of the C_xH_{10} monomers and binary complexes

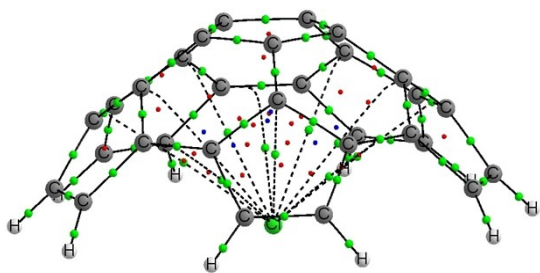
	<p>C₂₀H₁₀, M06-2X Energy= -768.005761964 Hartree</p> <p>C,0.7084348957,0.9750769902,-0.6451861008 C,1.4528830324,1.9997219377,-0.1063382125 C,0.6898518804,3.1720056359,0.2578017001 C,-0.6901419306,3.1719425916,0.2572747981 C,1.1460562682,-0.3721278305,-0.6451733406 C,2.3507567185,-0.7638942712,-0.1069642859 C,3.2299622512,0.3238201724,0.2572747929 C,2.8035806734,1.6362917646,0.2578016985 C,-0.0001212473,-1.2044885605,-0.6445031262 C,-0.0000753669,-2.4717071401,-0.1065116874 C,1.3062563722,-2.9718339742,0.2567201691 C,2.4226191125,-2.1607869892,0.2565389055 C,-1.1454992358,-0.3723227444,-0.6445031214 C,-2.3507098959,-0.7638711914,-0.1065116768 C,-2.4225024934,-2.1604258972,0.2581679229 C,-1.3060926851,-2.9715450983,0.2581679186 C,-0.7080654675,0.9749704577,-0.6451733357 C,-1.4529303958,1.9996461881,-0.1069642782 C,-2.8036610206,1.6363277975,0.2565389086 C,-3.2300374872,0.323976433,0.2567201672 H,-3.4786759136,2.4008890174,0.6287373217 H,-4.2252762287,0.1025084335,0.629785414 H,-3.3578999609,-2.565577564,0.6318615777 H,-1.4023610927,-3.986359713,0.6318615612 H,1.4031734619,-3.9867996305,0.6297854505 H,3.3583511254,-2.5665018749,0.6287373109 H,4.2250225261,0.1013491961,0.6304820859 H,3.4780644702,2.4005235635,0.631458418 H,1.2082525643,4.0496384505,0.6314584286 H,-1.2092149303,4.0495538497,0.6304820741</p>
	<p>C₃₀H₁₀, M06-2X Energy= -1148.87720150 Hartree</p> <p>C,0.7163207428,0.9859935649,-1.7057631355 C,1.3838548315,1.9053909326,-0.9397459963 C,0.6924702473,2.9559576215,-0.2225243982 C,-0.6924702023,2.9559576166,-0.2225242641 C,1.1593561988,-0.3769467325,-1.7056361175 C,2.2399128548,-0.7277765118,-0.9396696917 C,3.0229320945,0.2547413766,-0.2195629806 C,2.5949089455,1.5717410868,-0.2200057023 C,0.0000000536,-1.2194577007,-1.7057049434 C,-0.0000000228,-2.3563717265,-0.9408978762 C,1.1766013131,-2.7981917497,-0.2218797412 C,2.2967940024,-1.9835763798,-0.2214289961 C,-1.1593561635,-0.3769467271,-1.7056363092 C,-2.2399129279,-0.7277765462,-0.9396700171 C,-2.2967943188,-1.9835765108,-0.2214295988 C,-1.1766015784,-2.7981918644,-0.2218801824 C,-0.7163206409,0.9859936038,-1.7057631564 C,-1.3838547613,1.9053909886,-0.9397460138 C,-2.5949088288,1.5717409039,-0.2200056992 C,-3.0229320263,0.254741281,-0.2195630352 C,-2.7621362867,2.6505432039,0.7705762444 C,-3.7908094583,-0.5192590277,0.7726223493 C,-3.372304301,-1.8091671041,0.7716391213</p>

	<p>C,-0.6782123553,-3.7690359944,0.7692487355 C,0.6782118413,-3.7690359019,0.7692490327 C,3.372304217,-1.8091669315,0.7716394604 C,3.7908096125,-0.5192589964,0.7726223311 C,2.7621364135,2.6505436584,0.7705759763 C,1.6657750283,3.4483478694,0.7690072775 C,-1.6657749538,3.4483475601,0.7690076594 H,-3.6000375082,2.7399285461,1.4491081747 H,-4.5204142225,-0.0992362248,1.4522731805 H,-3.7166998777,-2.5789263296,1.4494688373 H,-1.3039743504,-4.3369069294,1.4449348141 H,1.3039735694,-4.3369067971,1.4449353582 H,3.7167000806,-2.5789260363,1.4494691767 H,4.5204149602,-0.0992364624,1.4522727056 H,3.6000376202,2.7399293631,1.4491078393 H,1.4920707454,4.2742933613,1.4458335993 H,-1.4920705879,4.2742926381,1.445834438</p>
	<p>C₄₀H₁₀, M06-2X Energy= -1529.91300721 Hartree</p> <p>C,0.7244714022,0.9975033907,-2.4725929242 C,1.4046040021,1.9334078527,-1.7213544179 C,0.6959567,2.9255745622,-0.9539418484 C,-0.6961806704,2.9262820085,-0.9553326444 C,1.1723683121,-0.3809425295,-2.4728465946 C,2.2726771753,-0.7385650158,-1.7217953965 C,2.9968870044,0.2418984851,-0.9536508772 C,2.5668892735,1.5656433034,-0.9529408033 C,0.0000161586,-1.2327062156,-2.4728465716 C,0.0001212112,-2.3896735699,-1.7217953809 C,1.1572411377,-2.776847598,-0.9552537812 C,2.2833317744,-1.9586948135,-0.9552537823 C,-1.1725560685,-0.3807677337,-2.4725929756 C,-2.2728266753,-0.7384019188,-1.721354535 C,-2.2822276474,-1.9574463489,-0.9529408301 C,-1.1561481257,-2.7754581087,-0.9536508378 C,-0.7247307315,0.9975063013,-2.4730825333 C,-1.405418866,1.9343931134,-1.7235215588 C,-2.5679279297,1.566377988,-0.9553326806 C,-2.9974492298,0.2421580487,-0.9539419579 C,-2.6411182109,2.3542560773,0.2252332142 C,-3.5177995027,-0.3505996201,0.2283929131 C,-3.0520817536,-1.7828905821,0.2289689468 C,-0.7520233714,-3.4554460439,0.22731966 C,0.7541769429,-3.4568456866,0.2259059594 C,3.054602073,-1.7854889818,0.2259059409 C,3.518712609,-0.352574875,0.2273195827 C,2.6387748226,2.3517586908,0.228969025 C,1.4204998233,3.2372848517,0.2283930429 C,-1.4228802536,3.2393577812,0.2252332083 C,-3.3508777955,1.8376993025,1.3002830842 C,-3.7885286072,0.4864401389,1.3021124028 C,-2.7780635406,-2.6176077825,1.3036746148 C,-1.6293364865,-3.4529841309,1.3027184883 C,1.6335179755,-3.4563786274,1.2998395227 C,2.7824265737,-2.6216476732,1.2998395067 C,3.7874759737,0.4825602798,1.3027183654 C,3.3479619307,1.8332100767,1.3036745977 C,0.7080875483,3.7534231133,1.3021124759 C,-0.7122778338,3.7547545152,1.3002830607 H,-3.4075368692,2.3859106157,2.2353061465</p>

	<p>H,-4.1547337045,0.078333948,2.2387852641 H,-3.3150633313,-2.5022916521,2.2399647425 H,-1.3523211346,-3.9280803604,2.2384528804 H,1.3576784565,-3.9324607232,2.2353920979 H,3.3204466836,-2.5064261326,2.2353920598 H,4.153716982,0.0722901756,2.2384526935 H,3.4042318465,2.3795618335,2.2399647482 H,1.2093831402,3.9755930836,2.2387853665 H,-1.2161491933,3.9780471868,2.23530608</p>
	<p>C₅₀H₁₀, M06-2X Energy= -1910.95519174 Hartree</p> <p>C,-0.0002693956,1.233343442,-2.9102435801 C,-0.0002026536,2.3982447049,-2.1547093385 C,-1.1566766378,2.7613459865,-1.3728282578 C,-2.2694422349,1.9540789957,-1.3735157609 C,1.1731145135,0.3810732696,-2.9104299698 C,2.2807744093,0.7411113372,-2.1546291932 C,2.2683835236,1.953415382,-1.3724121493 C,1.1567942502,2.7618674735,-1.3727118081 C,0.7250803516,-0.9978340577,-2.9104298964 C,1.409570992,-1.940177155,-2.1546291268 C,2.5592252096,-1.5542657774,-1.3728499277 C,2.9840311405,-0.2468474095,-1.3728500011 C,-0.7251590104,-0.9976374052,-2.9102436647 C,-1.4098167676,-1.9401016262,-2.1547094799 C,-0.6875186205,-2.9143441077,-1.372711737 C,0.686972069,-2.9136684447,-1.3724120264 C,-1.1733003073,0.3812284181,-2.9104940125 C,-2.2820149397,0.7414715769,-2.1558366439 C,-2.9845959749,-0.2469385699,-1.3735157521 C,-2.5588494434,-1.5540985117,-1.372828389 C,-3.4127748525,0.3508832791,-0.1320219306 C,-2.5543964128,-2.2891816945,-0.1313559453 C,-1.3878515566,-3.1363579578,-0.1310180884 C,1.3881138845,-3.137146345,-0.1312828106 C,2.5544360466,-2.2896880526,-0.1313254908 C,3.4124271283,0.3509366377,-0.1313256367 C,2.9669761865,1.7220917934,-0.1312829162 C,0.7207094709,3.3531255254,-0.1310180301 C,-0.721002947,3.3534234721,-0.1313558605 C,-2.9672368802,1.722108049,-0.1320219031 C,-3.5060591631,-0.3672116668,1.0574352497 C,-3.0526669897,-1.7630430611,1.057744915 C,-0.7339221728,-3.4474713129,1.0586456629 C,0.7338826468,-3.4480489375,1.058593558 C,3.0523427619,-1.763625917,1.0580326426 C,3.5060305948,-0.3673187465,1.0580325267 C,2.6204359173,2.3581645741,1.058593529 C,1.4326172724,3.2204512688,1.0586457068 C,-1.433368762,3.2206443328,1.0577450496 C,-2.6206199253,2.3578902334,1.0574352704 C,-3.5403799183,0.43033638,2.2547536814 C,-2.611988545,-2.4284794595,2.2552881703 C,-1.5039405372,-3.2331136894,2.2556974422 C,1.5042441656,-3.2350540659,2.2555263714 C,2.6120604709,-2.4299672208,2.2551294276 C,3.5415008616,0.4305541466,2.2551292519 C,3.1184765685,1.7330410747,2.2555262681 C,0.6836631716,3.4996380183,2.2556974784 C,-0.6857185922,3.499693732,2.2552882687</p>

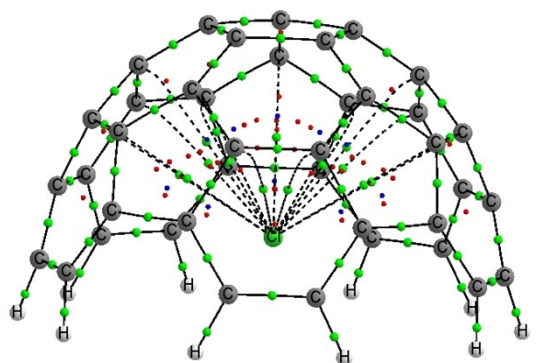
	<p>C,-3.1171731914,1.7328335776,2.2547536394 H,-3.7783846197,-0.0338583145,3.205411013 H,-3.0769020125,-2.1916390399,3.2058701342 H,-1.1353290405,-3.6017310528,3.2065004166 H,1.1372124896,-3.6055086351,3.2061910742 H,3.0783383236,-2.194362484,3.2054237579 H,3.7802433394,-0.0341251076,3.2054234895 H,3.0392896772,2.2484810565,3.206190929 H,1.1985440051,3.5811912354,3.2065004479 H,-1.2010528781,3.5816305648,3.2058702096 H,-3.03687646,2.248270705,3.2054109416</p>
	<p>C₆₀H₁₀, M06-2X Energy= -2291.99323607 Hartree</p> <p>C,-1.1726754392,-0.380907809,-3.5293615884 C,-2.2841088484,-0.7421100562,-2.7779806084 C,-2.2684881437,-1.9536084501,-1.9925320402 C,-1.1572653359,-2.759953836,-1.9920797534 C,-0.7248577704,0.9976811281,-3.5294916867 C,-1.4120811204,1.9435629232,-2.7785250889 C,-2.5584469546,1.5529744218,-1.9921252388 C,-2.9820877056,0.246858879,-1.9918366795 C,0.7246414918,0.9975736315,-3.5293615882 C,1.4116170562,1.9429919881,-2.7779806117 C,0.6867390354,2.9124175386,-1.9918366852 C,-0.6863628547,2.9131231379,-1.9921252439 C,1.1728634817,-0.3812425851,-3.5295404644 C,2.2841032222,-0.7419749001,-2.7777262378 C,2.9825262416,0.2477392622,-1.9920797464 C,2.5589934338,1.5537622254,-1.9925320401 C,0.0001484966,-1.2332698963,-3.5295404674 C,-0.0001666501,-2.4015941103,-2.7777262416 C,1.1565464511,-2.7599130145,-1.9914404945 C,2.2674407413,-1.9528010652,-1.9914404922 C,0.7067479824,-3.3444370728,-0.7439637789 C,2.9623515154,-1.7056451661,-0.7439637717 C,3.4003651769,-0.3600780516,-0.7447415607 C,2.5392965293,2.2908757275,-0.7450999852 C,1.3939895437,3.1217981132,-0.7446575731 C,-1.3933093122,3.1212694571,-0.7444393254 C,-2.5379473948,2.2896412094,-0.7444393219 C,-3.3997728739,-0.3610741715,-0.7446575635 C,-2.9634380559,-1.707094984,-0.7450999819 C,-0.7083160545,-3.3452097193,-0.7447415723 C,1.4113248048,-3.1812893036,0.4609807297 C,2.5894625489,-2.3253221136,0.4609807338 C,3.4662874977,0.3613653393,0.4599513555 C,3.015544843,1.7458267656,0.4596997006 C,0.7284091413,3.405448323,0.460109274 C,-0.727451002,3.404379601,0.4602704521 C,-3.01296266,1.7438581665,0.4602704602 C,-3.4638645859,0.3595831395,0.4601092845 C,-2.5922345217,-2.3284634541,0.4596996986 C,-1.4148206109,-3.1849673143,0.4599513447 C,0.7087525568,-3.3825151597,1.6838958847 C,2.9979464543,-1.7193184022,1.6838958917 C,3.4388212248,-0.3686709084,1.6833963045 C,2.565493613,2.3217452475,1.6829286737 C,1.4157198663,3.1560330592,1.6831938496 C,-1.4133433231,3.1537547348,1.6835757071 C,-2.5626518639,2.3187331938,1.683575712</p>

	<p>C,-3.4390472486,-0.3711617628,1.6831938565 C,-3.0008920476,-1.7224706987,1.6829286763 C,-0.7120273397,-3.3844389655,1.6833962948 C,1.4673969081,-3.1709554271,2.9009104583 C,2.5623072019,-2.3754565138,2.9009104615 C,3.4746954318,0.418456473,2.900310245 C,3.0564725052,1.7053498531,2.8999714842 C,0.6778034386,3.4305066258,2.9005589997 C,-0.6753245973,3.4292422202,2.9006403333 C,-3.052716335,1.7019659779,2.9006403409 C,-3.4720583947,0.4154554585,2.9005590084 C,-2.5663860312,-2.379896045,2.8999714838 C,-1.4717157043,-3.1753216307,2.9003102362 H,1.1016235747,-3.5674659135,3.840705205 H,3.0524412534,-2.1501138735,3.8407052099 H,3.7391652217,-0.0520854379,3.8399323033 H,2.9929047535,2.2422568173,3.8391029641 H,1.2071463669,3.5353879598,3.8402226296 H,-1.2047971029,3.5330091218,3.8405182998 H,-2.9877885149,2.2375899876,3.8405183087 H,-3.7353824181,-0.0555694719,3.8402226401 H,-3.0573713749,-2.1535261386,3.8391029661 H,-1.1059294156,-3.5722528054,3.8399322908</p>
	<p>C₂₀H₁₀:Cl⁻, M06-2X Energy= -1228.28753588 Hartree</p> <p>C,0.7087151149,0.9755672754,-0.7313023905 C,1.4448214527,1.9888678215,-0.1564267651 C,0.687968994,3.149634553,0.2396983481 C,-0.688596786,3.1496961373,0.239022412 C,1.1469407655,-0.3723967981,-0.7317883921 C,2.3376918079,-0.7593299803,-0.156092543 C,3.2080495666,0.3189174812,0.2397534663 C,2.7829618736,1.6281628166,0.2392587307 C,0.0001018392,-1.2055359885,-0.7318463229 C,-0.000092571,-2.457512403,-0.1559826395 C,1.2942910539,-2.9522536081,0.2398579711 C,2.4079866027,-2.1432303219,0.2398391927 C,-1.1468267124,-0.3724352736,-0.7326048967 C,-2.3379637405,-0.7592800178,-0.157450667 C,-2.4081276926,-2.14295084,0.2396050638 C,-1.2944538795,-2.9518150444,0.2404458499 C,-0.7087292717,0.9757644835,-0.7322310665 C,-1.4451756745,1.9890200404,-0.1575956487 C,-2.7829877902,1.6282416474,0.2383838158 C,-3.2081751574,0.3189543145,0.2385998592 H,-3.4311612288,2.3873474019,0.6670225683 H,-4.1785854487,0.0856675292,0.6676352905 H,-3.3308920119,-2.5248487854,0.667399874 H,-1.3723048166,-3.9472078922,0.6687187755 H,1.3723962725,-3.9479695349,0.6672057063 H,3.3309740046,-2.5254336585,0.6667439633 H,4.1793252157,0.0854083101,0.6668209021 H,3.4319591217,2.3877901581,0.6659025186 H,1.2096540195,4.0012467723,0.6674347188 H,-1.2106874927,4.0011281313,0.6665256021 Cl,0.0009225698,-0.0092147271,2.4972742192</p>



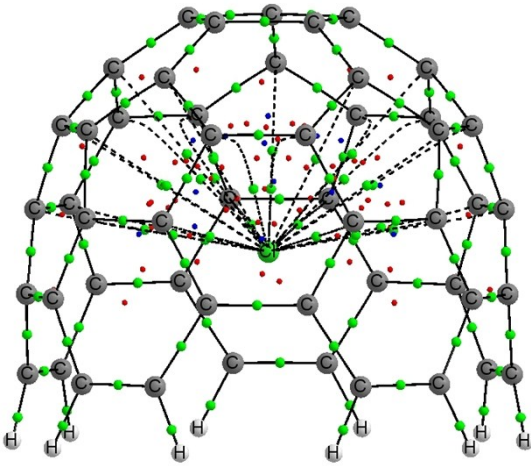
$C_{30}H_{10}:Cl^-$, M06-2X Energy= -1609.17747884 Hartree

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 C,-3.7606533664,-0.5088138628,0.7761554945
 C,-3.3416475021,-1.7977516823,0.7764820072
 C,-0.677436517,-3.7324577561,0.7775036605
 C,0.6778161696,-3.7317006816,0.7780399097
 C,3.3419375321,-1.7975905236,0.776143203
 C,3.7609040699,-0.5088671363,0.7753219818
 C,2.7420320552,2.6205999546,0.7775393271
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 H,-3.5525970275,2.6723823095,1.4931020705
 H,-4.4481610502,-0.074672401,1.4903373697
 H,-3.6425596486,-2.5527950562,1.4909789169
 H,-1.3028508836,-4.2497643286,1.4934202279
 H,1.303248551,-4.2480187286,1.4944941515
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 H,4.4488295737,-0.0742967386,1.4891254005
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 H,1.4440620216,4.2029616159,1.4940078014
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 Cl,0.001988463,0.0005617771,1.6215668761

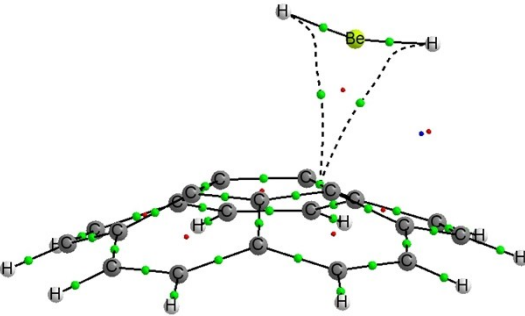


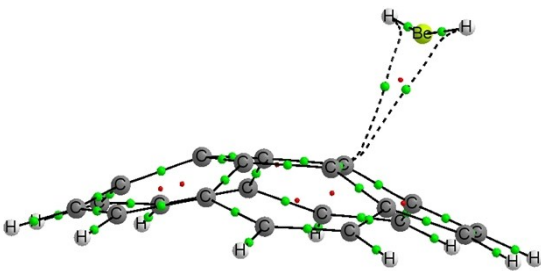
$C_{40}H_{10}:Cl^-$, M06-2X Energy= -1990.23477493 Hartree

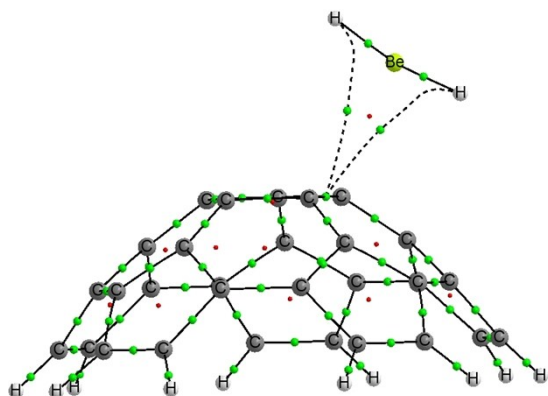
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 C,-2.284074686,-1.9598695666,-0.9805189663

	<p>C,-1.1577861822,-2.778157987,-0.9801375386 C,-0.7241266489,0.9966871202,-2.4894671768 C,-1.4062806419,1.9355766831,-1.7450198 C,-2.5693160317,1.5666035953,-0.9792122824 C,-2.9996086134,0.2428088939,-0.9800123993 C,-2.634524461,2.3475937043,0.2056460103 C,-3.5111211393,-0.3515584672,0.2045375409 C,-3.0473021019,-1.7804093808,0.2040980158 C,-0.7515357188,-3.4486441115,0.2047207499 C,0.7507932866,-3.4478450926,0.2055676207 C,3.0471426116,-1.7794739607,0.2049800176 C,3.512463342,-0.350961409,0.2042260672 C,2.6357626706,2.3484782801,0.2039863588 C,1.4198615305,3.2309130118,0.2049301405 C,-1.4188252409,3.2305856047,0.2060328519 C,-3.3256546637,1.8249426857,1.2878993318 C,-3.762895908,0.4762468169,1.2873988865 C,-2.7642681997,-2.5981410622,1.2869033884 C,-1.6173513024,-3.4316846435,1.2873032069 C,1.6151297401,-3.428440721,1.2892641779 C,2.7623820703,-2.5954877177,1.2887191118 C,3.7638547252,0.477649553,1.2867461875 C,3.3262611818,1.8259783632,1.2865541098 C,0.7098107007,3.7244583081,1.2882462398 C,-0.7079965542,3.724297759,1.2888300422 H,-3.3397020443,2.3561241309,2.2347357128 H,-4.0859500226,0.0535800888,2.2338089259 H,-3.2737159034,-2.4456970658,2.2334345199 H,-1.3167020332,-3.869284726,2.2343227427 H,1.3134233503,-3.865344629,2.2363405974 H,3.2716935261,-2.4427650977,2.2352449677</p>
	<p>C₅₀H₁₀:Cl, M06-2X Energy= -2371.29016988 Hartree</p> <p>C,0.0003316815,1.2335466736,-2.9123271888 C,0.0005066669,2.3990291458,-2.1595196117 C,-1.1563759052,2.7628126533,-1.3789900509 C,-2.2686232825,1.9548802371,-1.378932524 C,1.1721084909,0.3818303689,-2.9127734107 C,2.2803881013,0.7412846144,-2.15939221 C,2.2688283724,1.9534656551,-1.3785176508 C,1.1572010564,2.7623780586,-1.3788861547 C,0.7241972028,-0.995732936,-2.9132675892 C,1.4091238476,-1.9392558979,-2.1610821577 C,2.5590502051,-1.5544383705,-1.3805762315 C,2.9837918272,-0.2468714294,-1.3795580483 C,-0.724554973,-0.9955296217,-2.9130771098 C,-1.4096930268,-1.9385505241,-2.1605692533 C,-0.6879973904,-2.9132976659,-1.3807446405 C,0.6868402208,-2.9138837394,-1.3811977196 C,-1.172015183,0.3822052032,-2.9125765874 C,-2.2801513903,0.7424038898,-2.1593961782 C,-2.9838908836,-0.2454031552,-1.379354229 C,-2.5591733862,-1.5528861561,-1.3798180544 C,-3.4142535631,0.3530238639,-0.1398953298 C,-2.5554626873,-2.2906168433,-0.1407434521 C,-1.3903658856,-3.138209678,-0.141421405 C,1.3896439136,-3.1396701519,-0.1422543029 C,2.5556637425,-2.2928433546,-0.1418152417 C,3.4141656584,0.3511965917,-0.1399069323 C,2.9684768803,1.7214329888,-0.1391950366</p>

	<p>C,0.7209154865,3.3568093429,-0.1394659955 C,-0.720001616,3.357347506,-0.1396728186 C,-2.9692021805,1.7234339595,-0.1397372741 C,-3.5032288166,-0.3665321061,1.048331093 C,-3.0498040405,-1.7611003977,1.0479065771 C,-0.7332550548,-3.4454678594,1.0466665279 C,0.7330308186,-3.4467743755,1.0461294056 C,3.0501793075,-1.7636579433,1.0468790609 C,3.5024950201,-0.3688290434,1.0480312082 C,2.6175282897,2.3551535876,1.0493303972 C,1.4320414174,3.2178467543,1.0491252105 C,-1.4317238186,3.2193163282,1.0486466393 C,-2.6180519154,2.3575587225,1.0486599109 C,-3.5271903373,0.4273727922,2.2458771601 C,-2.6023872812,-2.4181429593,2.244969349 C,-1.4952889463,-3.223122823,2.2444432641 C,1.4960002423,-3.2254524565,2.2436228242 C,2.6035803492,-2.4212941005,2.24395466 C,3.5262842681,0.4244488485,2.2459353077 C,3.1034764033,1.7263504503,2.2465222604 C,0.6844629091,3.4864367066,2.2465664281 C,-0.6843219338,3.4873524567,2.2463167284 C,-3.10393384,1.7290801045,2.246109486 H,-3.7378749545,-0.043311512,3.2001079752 H,-3.0491525648,-2.1613155036,3.1994082035 H,-1.1129457571,-3.5689829574,3.1987337919 H,1.1139423511,-3.5720448101,3.1978044174 H,3.0511418859,-2.1656763213,3.1983350288 H,3.7363018658,-0.0467821247,3.2000725624 H,2.9969188844,2.2301555727,3.2011591752 H,1.1969338877,3.5411424363,3.2009453816 H,-1.1969849791,3.5430003319,3.2005499823 H,-2.997520683,2.2332181319,3.2006000761 Cl,-0.0001249776,0.0001628968,0.4564114924</p>
	<p>C₆₀H₁₀:Cl⁻, M06-2X Energy= -2752.33367041 Hartree</p> <p>C,1.1716565075,-0.3806876387,3.5046250521 C,2.2829760048,-0.7415989251,2.755058241 C,2.2671641916,-1.9523353115,1.9704842327 C,1.1567422568,-2.7595344139,1.9706148797 C,0.7237163967,0.9966154639,3.5044786461 C,1.4107246246,1.9422514176,2.7554582728 C,2.5572028432,1.5528494251,1.9707660523 C,2.9819556959,0.2472854888,1.9708369651 C,-0.7245561085,0.9968100679,3.5049904254 C,-1.4110580341,1.9419846355,2.7548474889 C,-0.6866431537,2.9127357485,1.9708930738 C,0.6863166236,2.9126654441,1.971000958 C,-1.1720183632,-0.3806210359,3.5043392729 C,-2.2832990316,-0.7417824792,2.7548715627 C,-2.9822549721,0.2470503856,1.9703821472 C,-2.5575898585,1.5526918981,1.9702964033 C,-0.0001147575,-1.232096122,3.5044254786 C,0.0000305338,-2.4006205381,2.7549991081 C,-1.1564449018,-2.7595635906,1.9703452129 C,-2.2669662988,-1.9525122195,1.9701227019 C,-0.7070017999,-3.3465300203,0.7251370837 C,-2.9629408498,-1.7064432968,0.7245397199 C,-3.4006196081,-0.361246755,0.724617945 C,-2.5387325592,2.2912032052,0.7249427883</p>

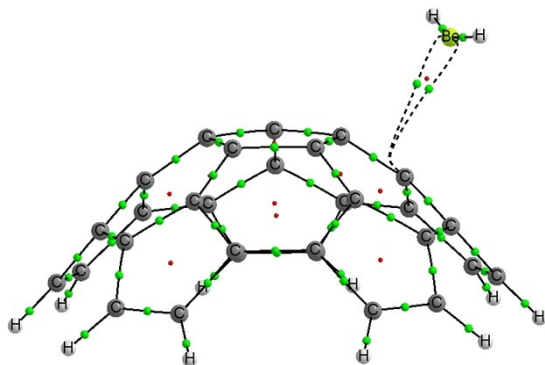
	<p>C,-1.3946805237,3.1233078907,0.7252634127 C,1.3946009498,3.123296594,0.7255305188 C,2.538847331,2.2915677884,0.7254664768 C,3.4009503643,-0.360915218,0.7252411974 C,2.9638839531,-1.7063453901,0.7250515341 C,0.7076525834,-3.3464293723,0.7251480849 C,-1.4131309403,-3.1839619327,-0.4781937403 C,-2.5899160005,-2.3279478435,-0.4785007815 C,-3.4635647584,0.3605883452,-0.4785743679 C,-3.0145320343,1.7447997565,-0.4783315568 C,-0.7275610979,3.4063157888,-0.4779481691 C,0.7276546498,3.4063588303,-0.4778049554 C,3.0146312169,1.7452277412,-0.4779827407 C,3.4638061121,0.3610345093,-0.4780770214 C,2.590960901,-2.3278017248,-0.4781077106 C,1.4135102406,-3.1834699421,-0.478125044 C,-0.709374326,-3.3837915551,-1.6994197343 C,-2.9983126635,-1.7209342655,-1.6997058894 C,-3.4363115383,-0.3706186089,-1.6997513434 C,-2.5633471897,2.3207710356,-1.6993350786 C,-1.4146710253,3.1552952512,-1.6992043567 C,1.4146658571,3.155305859,-1.6991161303 C,2.5631975284,2.3210585114,-1.6991850957 C,3.436272404,-0.3701383942,-1.6992287182 C,2.9985024384,-1.7204173433,-1.6992616253 C,0.709949674,-3.3837533802,-1.6994415644 C,-1.4640438216,-3.167076327,-2.9173163905 C,-2.5586426084,-2.3716442673,-2.9174949321 C,-3.4627116631,0.4140435828,-2.9175424716 C,-3.0449967872,1.7011140054,-2.9173123306 C,-0.6766347962,3.4219841235,-2.917140693 C,0.6765421798,3.4216497418,-2.9171400012 C,3.044600304,1.7011317804,-2.9173031725 C,3.461890277,0.4140794695,-2.9173096415 C,2.5586844814,-2.3706852035,-2.9171970715 C,1.4639900771,-3.1658413077,-2.9173618403 H,-1.0900966688,-3.5511551411,-3.8597893459 H,-3.0398004128,-2.1344761485,-3.8597919467 H,-3.7105232882,-0.0607788646,-3.8602796065 H,-2.9666971865,2.2313365736,-3.8599285509 H,-1.2048964756,3.5115143798,-3.8598565651 H,1.2047612249,3.5102523905,-3.8598674302 H,2.9662704223,2.2312333432,-3.8598919934 H,3.7094507479,-0.0611212292,-3.8598970194 H,3.0389758109,-2.1327699792,-3.8597076081 H,1.0896088517,-3.5489536641,-3.8600500386 Cl,0.0023398434,-0.0008110156,0.1170842085</p>
	<p>[65]BeH₂:C₂₀H₁₀, M06-2X Energy=-783.912236050 Hartree</p> <p>C,0.49385908,0.8818097727,0.7097127373 C,-0.0578550598,1.9029436468,1.4545381005 C,-0.4301015787,3.0688770375,0.6905033875 C,-0.4301015787,3.0688770386,-0.6905033825 C,0.5166254711,-0.4662402956,1.1445722225 C,-0.0121398523,-0.8643030865,2.3509940157 C,-0.3892634929,0.2200122218,3.2294630501 C,-0.4103222608,1.5336675259,2.8060959713 C,0.532450279,-1.2965537746,-0.000000001 C,0.015816095,-2.5731776244,-0.0000000021</p>

	<p>C,-0.3400548381,-3.0776906833,1.306317181 C,-0.3538715385,-2.2661285736,2.4231240086 C,0.5166254711,-0.4662402937,-1.1445722232 C,-0.0121398523,-0.8643030827,-2.3509940171 C,-0.3538715385,-2.2661285697,-2.4231240122 C,-0.3400548381,-3.0776906812,-1.3063171859 C,0.49385908,0.8818097738,-0.7097127359 C,-0.0578550598,1.9029436492,-1.4545380974 C,-0.4103222608,1.5336675305,-2.8060959688 C,-0.3892634929,0.220012227,-3.2294630498 H,-0.7891036928,2.2918277047,-3.4841767095 H,-0.7540060803,-0.0072792099,-4.2264359434 H,-0.7213758262,-2.6767850179,-3.3584764129 H,-0.6978226616,-4.0980214263,-1.4029892859 H,-0.6978226616,-4.0980214286,1.4029892793 H,-0.7213758262,-2.6767850234,3.3584764085 H,-0.7540060803,-0.0072792167,4.2264359434 H,-0.7891036928,2.2918276991,3.4841767132 H,-0.8073625307,3.9455142775,1.2074480319 H,-0.8073625307,3.9455142794,-1.2074480255 Be,2.8544064362,1.6018453705,0.0000000013 H,3.4157029599,0.3889735864,0.0000000003 H,2.6578841196,2.9250352323,0.0000000024</p>
	<p>[66]BeH₂:C₂₀H₁₀, M06-2X Energy=-783.911749387 Hartree</p> <p>C,0.5053304708,1.2248052079,0. C,-0.1126437606,2.4610192179,0. C,-0.4905756379,2.9424233611,-1.3090797046 C,-0.4351036223,2.131842529,-2.4247254678 C,0.5500442609,0.3917855742,1.1472001315 C,-0.0004790657,0.7562679962,2.3535899124 C,-0.4351036223,2.131842529,2.4247254678 C,-0.4905756379,2.9424233611,1.3090797046 C,0.6250614252,-0.9500386209,0.7080096763 C,0.1454090541,-2.0030506588,1.4543066721 C,-0.2314780404,-1.6595897838,2.8070089642 C,-0.3004061123,-0.3495305872,3.2349849823 C,0.6250614252,-0.9500386209,-0.7080096763 C,0.1454090541,-2.0030506588,-1.4543066721 C,-0.1556752641,-3.1915052061,-0.6904958516 C,-0.1556752641,-3.1915052061,0.6904958516 C,0.5500442609,0.3917855742,-1.1472001315 C,-0.0004790657,0.7562679962,-2.3535899124 C,-0.3004061123,-0.3495305872,-3.2349849823 C,-0.2314780404,-1.6595897838,-2.8070089642 H,-0.6773131809,-0.148655064,-4.2329142302 H,-0.5582327855,-2.443626864,-3.4829956856 H,-0.4809255483,-4.0883873872,-1.2085364376 H,-0.4809255483,-4.0883873872,1.2085364376 H,-0.5582327855,-2.443626864,3.4829956856 H,-0.6773131809,-0.148655064,4.2329142302 H,-0.8159808873,2.5208168102,3.3640365527 H,-0.911457857,3.9377761122,1.4096103149 H,-0.911457857,3.9377761122,-1.4096103149 H,-0.8159808873,2.5208168102,-3.3640365527 Be,2.5583326764,2.5899025085,0. H,2.7469827692,2.6858386082,-1.3216621879 H,2.7469827692,2.6858386082,1.3216621879</p>



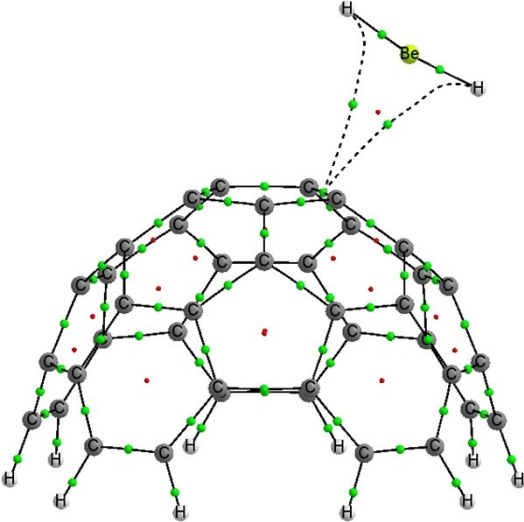
[65]BeH₂:C₃₀H₁₀, M06-2X Energy= -1164.78134902 Hartree

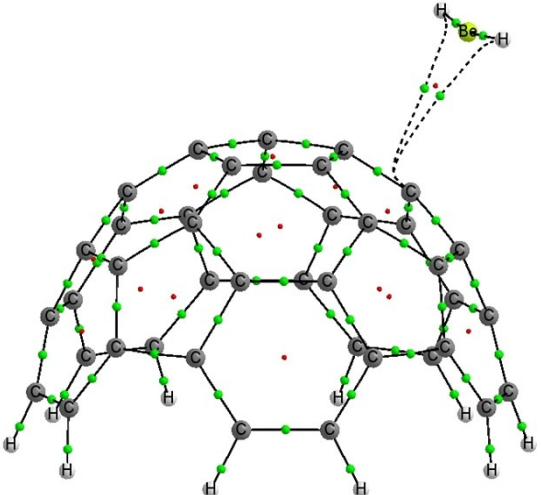
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 C,-3.3705123345,-1.8079985231,0.7632229159
 C,-0.6737063033,-3.7638070525,0.7625626408
 C,0.6819440851,-3.7643458906,0.7609796337
 C,3.3812765692,-1.8085558241,0.7538665504
 C,3.8013402347,-0.5196921929,0.7526327045
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 H,1.3098787736,-4.3278830725,1.438247618
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 H,3.6118032899,2.749057142,1.4253893415
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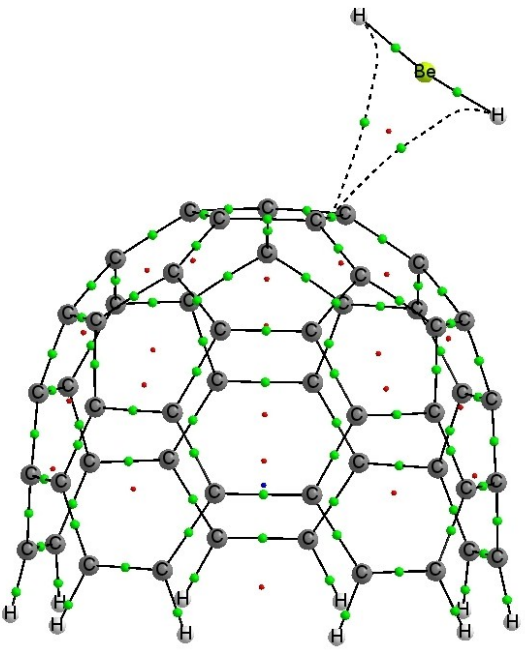


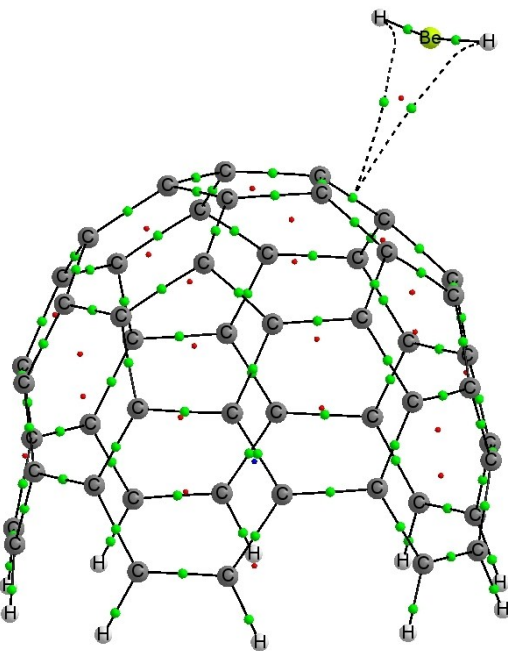
[66]BeH₂:C₃₀H₁₀, M06-2X Energy -1164.78166328 Hartree

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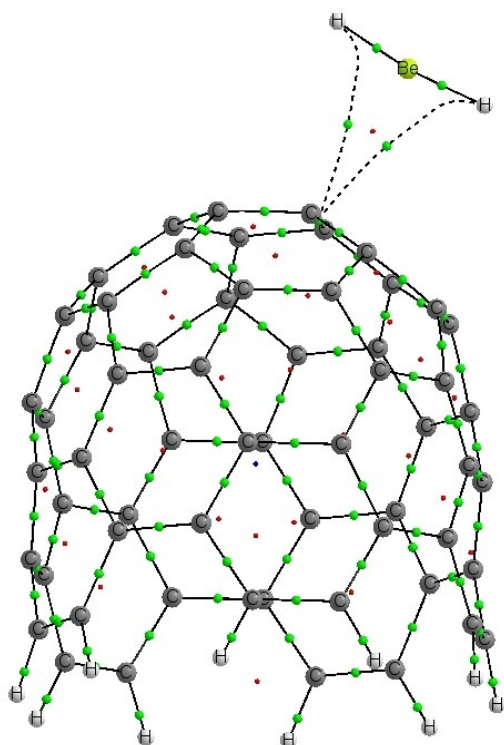
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	<p>[65]BeH₂:C₄₀H₁₀, M06-2X Energy=-1545.81675095 Hartree</p> <p>C,0.6633202256,0.978612333,-2.5032165394 C,1.3585656677,1.9178175759,-1.7689804303 C,0.6620136717,2.917368936,-0.9997844593 C,-0.7298534701,2.9152137528,-0.9794878114 C,1.1118512331,-0.40182416,-2.5032165394 C,2.2263676023,-0.753002143,-1.7689804303 C,2.9634846014,0.2316340279,-1.0195329302 C,2.5336604677,1.554496684,-1.0195329302 C,-0.0611345598,-1.2526079658,-2.4861523806 C,-0.0469383976,-2.4055791801,-1.730355967 C,1.1230557958,-2.7874545721,-0.9794878114 C,2.2503667508,-1.9710791707,-0.9997844593 C,-1.2328565282,-0.40057937,-2.4721258139 C,-2.3202407038,-0.7538919071,-1.6999468587 C,-2.3160758372,-1.9688408494,-0.9255525368 C,-1.1903876936,-2.7878779703,-0.9416161768 C,-0.7857233889,0.9774471374,-2.4861523806 C,-1.4519379304,1.9185647373,-1.7303559671 C,-2.6017174331,1.5557483203,-0.9416161768 C,-3.0310003284,0.2314704802,-0.9255525368 C,-2.6556479258,2.3501734747,0.2355126808 C,-3.5312845576,-0.3553257838,0.2687050606 C,-3.065724471,-1.7881723929,0.2687050606 C,-0.7670669877,-3.4622809683,0.2355126808 C,0.738559311,-3.4625216866,0.2106221509</p>

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	<p>[66]BeH₂:C₄₀H₁₀, M06-2X Energy=-1545.8155318 Hartree</p> <p>C,0.7158037056,0.9852192802,-2.4811357947 C,1.3996023021,1.926387307,-1.7347178543 C,0.6932282982,2.9254366008,-0.9734057598 C,-0.6980221559,2.9248414147,-0.9725025534 C,1.1674317258,-0.3912061596,-2.4842983651 C,2.2699733684,-0.7435452127,-1.7346203911 C,2.9973901949,0.2399671868,-0.9725025534 C,2.5680362152,1.5633089191,-0.9734057598 C,-0.0055454051,-1.2407989164,-2.4807839203 C,-0.0035492012,-2.3957679883,-1.7271354252 C,1.1548570357,-2.7784282003,-0.9596888389 C,2.2816374728,-1.9611187163,-0.9640158141 C,-1.1783562699,-0.3887019469,-2.4807839203 C,-2.2774139924,-0.7437085167,-1.7271354252 C,-2.2855467535,-1.9613957615,-0.9568936941 C,-1.1591254284,-2.7797887576,-0.9568936941 C,-0.7328154115,0.9894041977,-2.4842983651 C,-1.4086138696,1.9291048553,-1.7346203912 C,-2.5701994903,1.5639471718,-0.9640158141 C,-2.9993126954,0.239752774,-0.959688839 C,-2.6394210883,2.3539719949,0.2155603821 C,-3.5174985188,-0.3513139598,0.2243582699 C,-3.0535482511,-1.7842568527,0.2259054909 C,-0.7533307996,-3.4554626528,0.2259054909 C,0.7528473935,-3.4539018704,0.2243582699 C,3.0543863787,-1.7828212708,0.2155603822 C,3.5207821253,-0.350305671,0.2098907393 C,2.6430463131,2.3559557994,0.2032867639 C,1.4239008834,3.2417168007,0.2032867638</p>

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	<p>[65]BeH₂:C₅₀H₁₀, M06-2X Energy=-1926.85892799 Hartree</p> <p>C,-0.0095458699,1.2223149802,-2.9170322041 C,-0.0053330293,2.3910729189,-2.1670111118 C,-1.1621778377,2.7593993806,-1.3872682014 C,-2.2721189092,1.9480121246,-1.3826801854 C,1.165434611,0.3686564471,-2.9170321323 C,2.275681562,0.7338474573,-2.1670109724 C,2.2662561621,1.9500650032,-1.3919366563 C,1.1542651085,2.7579598295,-1.3919367243 C,0.7162292198,-1.009694653,-2.9175958173 C,1.4035472963,-1.9487802104,-2.1618566327 C,2.5548186944,-1.5589027057,-1.3826798905 C,2.9834817025,-0.2525465191,-1.387267948 C,-0.7331765655,-1.0091486316,-2.9159275106 C,-1.4166693842,-1.9499119875,-2.157086673 C,-0.6921350689,-2.9214122316,-1.374091099 C,0.6830057077,-2.9211822682,-1.376592103 C,-1.1816095401,0.3691420835,-2.9175959333 C,-2.2871319807,0.7326088925,-2.1618568582 C,-2.9892655556,-0.2531671389,-1.3765923273 C,-2.5645208934,-1.5610678155,-1.3740912134 C,-3.4133581098,0.3482791204,-0.13515919 C,-2.5569796189,-2.2926604628,-0.130419432 C,-1.3902479062,-3.1403260185,-0.1304193607 C,1.386070374,-3.13864951,-0.1351588968 C,2.5522139226,-2.2907968238,-0.1391043442 C,3.4125122214,0.3499523725,-0.1483388528 C,2.9674852975,1.721936623,-0.1519462121 C,0.7206005025,3.3543657648,-0.1519463493 C,-0.7217549299,3.3536213602,-0.1483391054 C,-2.9673830013,1.7193557614,-0.1391046815 C,-3.5042498402,-0.3670986578,1.0562093167 C,-3.0524320094,-1.7635730371,1.0586400346 C,-0.7339476904,-3.4480213788,1.0586401763</p>

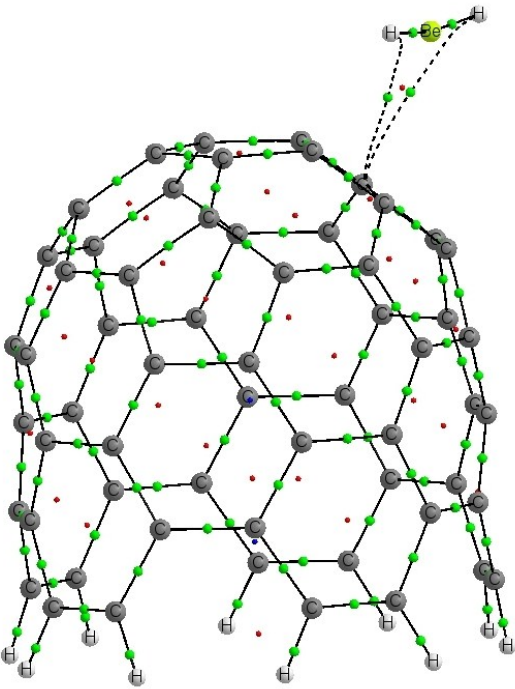
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	<p>[66]BeH₂:C₅₀H₁₀, M06-2X Energy=-1926.85820431 Hartree</p> <p>C,-0.0000000164,1.2322938603,-2.910988465 C,-0.0000000229,2.3996487724,-2.1544202567 C,-1.1588402499,2.7682780739,-1.3782384053 C,-2.270142746,1.959632996,-1.3808309716 C,1.1751473043,0.3834717675,-2.9165683362 C,2.2822248027,0.746231839,-2.1623392245 C,2.2701427106,1.959633029,-1.3808309836 C,1.1588402028,2.7682780908,-1.3782384114 C,0.7252084011,-0.9940797294,-2.9178346713 C,1.410145642,-1.9361143141,-2.1630269789 C,2.5599305492,-1.5493228004,-1.3803905379 C,2.9851330632,-0.2419941231,-1.3800746762 C,-0.7252084015,-0.9940797399,-2.9178346674 C,-1.4101456248,-1.9361143346,-2.1630269715 C,-0.6875305974,-2.9102242006,-1.3820386046 C,0.6875306328,-2.9102241906,-1.3820386082 C,-1.1751473248,0.3834717504,-2.91656833 C,-2.2822248245,0.7462318058,-2.1623392124 C,-2.9851330666,-0.2419941665,-1.3800746605 C,-2.5599305335,-1.5493228376,-1.3803905244 C,-3.4125333607,0.3558648164,-0.1388884956 C,-2.5544216252,-2.2853857879,-0.1394048196 C,-1.3879667781,-3.1331466716,-0.1403221615 C,1.3879668234,-3.1331466514,-0.1403221689 C,2.5544216582,-2.2853857508,-0.1394048331 C,3.4125333553,0.3558648661,-0.1388885136 C,2.9686257386,1.728096963,-0.1394499514</p>

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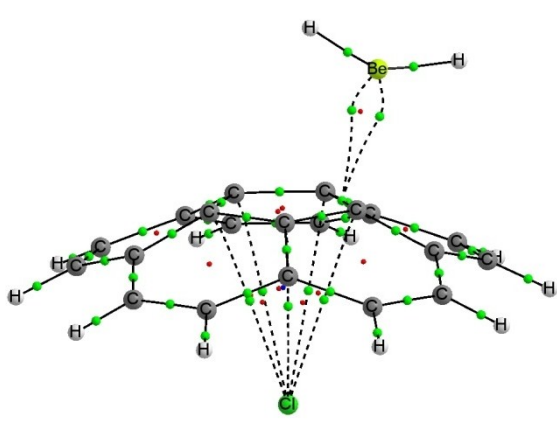
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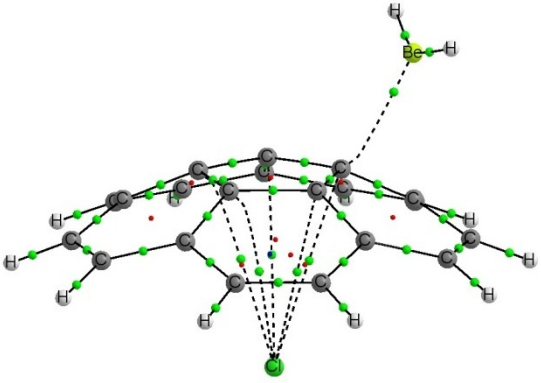
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 C,0.0301939708,4.4121571679,-1.4679872985
 C,0.0301939708,4.4121571679,1.4679872985
 C,0.5733732316,3.8298556711,2.5621949465
 C,2.4755135825,1.7836830873,3.4759867447

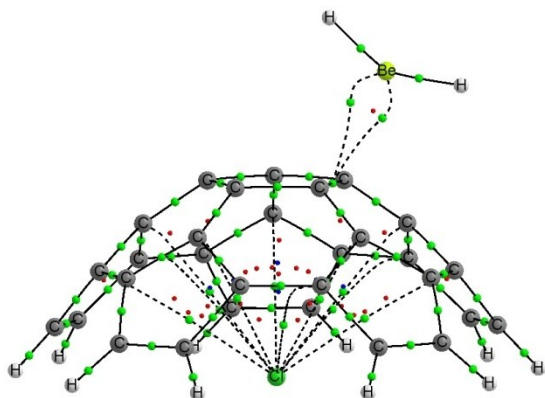
	<p>C,3.3522707141,0.8415682107,3.0586331658 C,4.527024573,-0.418508829,0.6766131801 C,4.527024573,-0.418508829,-0.6766131801 H,4.406211875,1.0865991733,-2.9990583639 H,2.8415810158,2.7675185421,-3.7450274555 H,1.4171503448,4.3031414003,-3.0506324136 H,0.4479043781,5.3421130918,-1.1001973993 H,0.4479043781,5.3421130918,1.1001973993 H,1.4171503448,4.3031414003,3.0506324136 H,2.8415810158,2.7675185421,3.7450274555 H,4.406211875,1.0865991733,2.9990583639 H,5.2875330661,0.1423398435,1.2070570285 H,5.2875330661,0.1423398435,-1.2070570285 Be,-2.5697812825,-5.629356441,0. H,-1.316763598,-6.0823759252,0. H,-3.8745712988,-5.3577584807,0.</p>
	<p>[66]BeH₂:C₆₀H₁₀, M06-2X Energy=-2307.89566364 Hartree</p> <p>C,-1.1748392263,-0.3333810391,-3.5672922974 C,-2.2854672948,-0.7046248832,-2.8206004211 C,-2.2689644623,-1.9229810756,-2.0457261735 C,-1.1587272914,-2.7302637146,-2.0499929571 C,-0.7252988039,1.0445608443,-3.5548112326 C,-1.4119787486,1.9812713513,-2.7938277102 C,-2.5598023212,1.5826479569,-2.0121667125 C,-2.9853561428,0.2772243127,-2.0256559941 C,0.7252988039,1.0445608443,-3.5548112326 C,1.4119787486,1.9812713513,-2.7938277102 C,0.6867709632,2.9431236955,-1.9985196307 C,-0.6867709632,2.9431236955,-1.9985196307 C,1.1748392263,-0.3333810391,-3.5672922974 C,2.2854672948,-0.7046248832,-2.8206004211 C,2.9853561428,0.2772243127,-2.0256559941 C,2.5598023212,1.5826479569,-2.0121667125 C,0,-1.1811855877,-3.5689773743 C,0,-2.3606493933,-2.8284690488 C,1.1587272914,-2.7302637146,-2.0499929571 C,2.2689644623,-1.9229810756,-2.0457261735 C,0.7077704247,-3.3269505294,-0.8099336714 C,2.9660765248,-1.6894743821,-0.7968549379 C,3.402794356,-0.3432015654,-0.7842351107 C,2.5409101301,2.3085980891,-0.7581126105 C,1.3944770494,3.1388097777,-0.7492984082 C,-1.3944770494,3.1388097777,-0.7492984082 C,-2.5409101301,2.3085980891,-0.7581126105 C,-3.402794356,-0.3432015654,-0.7842351107 C,-2.9660765248,-1.6894743821,-0.7968549379 C,-0.7077704247,-3.3269505294,-0.8099336714 C,1.4134983131,-3.1760357203,0.3957001473 C,2.5931858874,-2.321239358,0.4017819295 C,3.4663972242,0.366267354,0.4270449286 C,3.0164251155,1.7510972021,0.4407052025 C,0.7279011792,3.4074865092,0.4575271126 C,-0.7279011792,3.4074865092,0.4575271126 C,-3.0164251155,1.7510972021,0.4407052025 C,-3.4663972242,0.366267354,0.4270449286 C,-2.5931858874,-2.321239358,0.4017819295 C,-1.4134983131,-3.1760357203,0.3957001473 C,0.7102094208,-3.3844971902,1.6174403317</p>

	C,3.0024617458,-1.7267605333,1.6307103786 C,3.4408292899,-0.3760083962,1.6430636046 C,2.5656600377,2.3138194676,1.6702350879 C,1.4149672618,3.1460895688,1.6786552343 C,-1.4149672618,3.1460895688,1.6786552343 C,-2.5656600377,2.3138194676,1.6702350879 C,-3.4408292899,-0.3760083962,1.6430636046 C,-3.0024617458,-1.7267605333,1.6307103786 C,-0.7102094208,-3.3844971902,1.6174403317 C,1.4703013606,-3.1860519699,2.8361997745 C,2.5671201708,-2.3938468706,2.8424139639 C,3.476260443,0.3991302329,2.8682176869 C,3.0575154898,1.6856242728,2.8810548643 C,0.6766564555,3.4079754789,2.8983003701 C,-0.6766564555,3.4079754789,2.8983003701 C,-3.0575154898,1.6856242728,2.8810548643 C,-3.476260443,0.3991302329,2.8682176869 C,-2.5671201708,-2.3938468706,2.8424139639 C,-1.4703013606,-3.1860519699,2.8361997745 H,1.1037462573,-3.590830086,3.7722355937 H,3.0590897553,-2.1770927845,3.7833502481 H,3.7416553998,-0.0807949097,3.8028222755 H,2.9925640802,2.2132463674,3.8255511648 H,1.2066672446,3.5013682017,3.8389077942 H,-1.2066672446,3.5013682017,3.8389077942 H,-2.9925640802,2.2132463674,3.8255511648 H,-3.7416553998,-0.0807949097,3.8028222755 H,-3.0590897553,-2.1770927845,3.7833502481 H,-1.1037462573,-3.590830086,3.7722355937 Be,0,-3.2415431515,-5.3805771251 H,-1.3273592826,-3.3130275741,-5.4969755029 H,1.3273592826,-3.3130275741,-5.4969755029
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Table S2. Molecular Graph; M06-2X energy, Cartesian coordinates of the minima geometry of the ternary systems

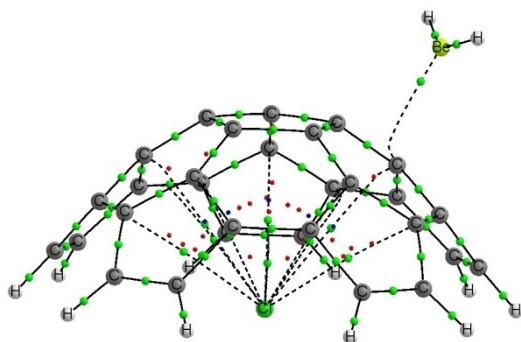
	[65] BeH ₂ :C ₂₀ H ₁₀ :Cl M06-2X Energy= - 1244.20389275 Hartree
	C,0.5816719086,0.8866752326,0.7125286885 C,-0.0225976489,1.8939754199,1.4446635746 C,-0.4321394724,3.0439567247,0.6886696979 C,-0.4321394749,3.0439566861,-0.6886698702 C,0.5921302306,-0.4654065561,1.1447992024 C,0.020706281,-0.8557590144,2.3362158922 C,-0.3889099144,0.2189824315,3.203715276 C,-0.4095061741,1.5291140302,2.7818961437 C,0.6037443153,-1.2951370567,0.0000000336 C,0.0379601492,-2.5537612278,0.0000000699 C,-0.3556347807,-3.0506272824,1.2925804055 C,-0.3644631278,-2.2411351259,2.4065372955 C,0.5921302264,-0.4654066203,-1.1447991817 C,0.0207062724,-0.8557591454,-2.3362158475 C,-0.3644631366,-2.2411352608,-2.4065371717 C,-0.3556347854,-3.0506273548,-1.2925802364 C,0.581671906,0.8866751926,-0.7125287435 C,-0.0225976542,1.8939753389,-1.4446636839

	<p>C,-0.4095061842,1.5291138743,-2.7818962311 C,-0.3889099261,0.2189822519,-3.2037152901 H,-0.8447539971,2.2825725088,-3.4311025692 H,-0.8105623352,-0.0202527063,-4.1757899574 H,-0.7904088413,-2.6255943246,-3.3287499706 H,-0.7761944019,-4.0489996475,-1.3699489133 H,-0.7761943969,-4.0489995707,1.3699491399 H,-0.7904088291,-2.625594138,3.3287501174 H,-0.8105623199,-0.0202524722,4.1757899583 H,-0.8447539846,2.2825727011,3.4311024411 H,-0.8709414478,3.8894664083,1.2096964528 H,-0.8709414523,3.8894663405,-1.2096966709 Be,2.6298520526,1.5363607867,-0.0000000495 H,3.4004324894,0.4247226058,-0.0000000197 H,2.6361001912,2.8901010905,-0.0000000874 Cl,-2.5929703946,-0.0573732851,0.0000000047</p>
	<p>[66] BeH₂:C₂₀H₁₀:Cl⁻ M06-2X Energy= - 1244.20344103 Hartree</p> <p>C,0.5949883808,1.2288632729,0. C,-0.0687604167,2.4476582295,0. C,-0.4799585147,2.9236026268,-1.2962829258 C,-0.4315122173,2.1128698909,-2.4066482758 C,0.6226890491,0.3904214632,1.1493291743 C,0.030896022,0.7517897466,2.3384892254 C,-0.4315122173,2.1128698909,2.4066482758 C,-0.4799585147,2.9236026268,1.2962829258 C,0.690933795,-0.9506441537,0.708933652 C,0.1629760638,-1.990169263,1.4461662665 C,-0.2477474432,-1.6496430939,2.7847801505 C,-0.3108929618,-0.3428452868,3.2110342554 C,0.690933795,-0.9506441537,-0.708933652 C,0.1629760638,-1.990169263,-1.4461662665 C,-0.1801740224,-3.1649648515,-0.688959808 C,-0.1801740224,-3.1649648515,0.688959808 C,0.6226890491,0.3904214632,-1.1493291743 C,0.030896022,0.7517897466,-2.3384892254 C,-0.3108929618,-0.3428452868,-3.2110342554 C,-0.2477474432,-1.6496430939,-2.7847801505 H,-0.7433962389,-0.1303187895,-4.184259364 H,-0.6335040816,-2.4300213851,-3.4342797068 H,-0.5697314837,-4.0349268823,-1.2098368744 H,-0.5697314837,-4.0349268823,1.2098368744 H,-0.6335040816,-2.4300213851,3.4342797068 H,-0.7433962389,-0.1303187895,4.184259364 H,-0.8675992866,2.4762651896,3.3326426836 H,-0.9507850544,3.8982627087,1.3760837611 H,-0.9507850544,3.8982627087,-1.3760837611 H,-0.8675992866,2.4762651896,-3.3326426836 Be,2.355195919,2.5359110646,0. H,2.7177567215,2.7297755628,-1.2895272923 H,2.7177567215,2.7297755628,1.2895272923 Cl,-2.5354755579,-0.0507060075,0.</p>



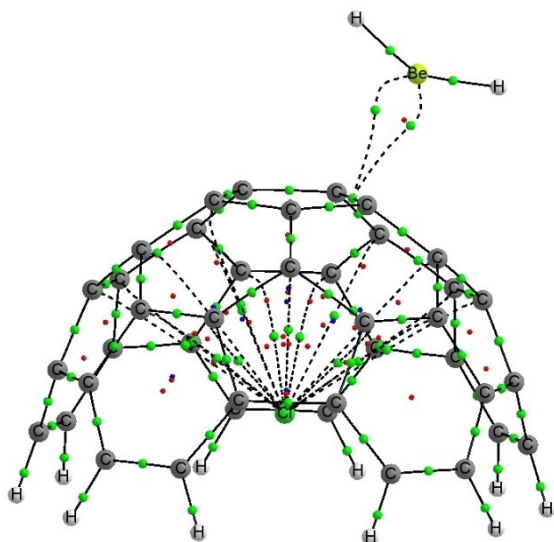
[65] BeH₂:C₃₀H₁₀:Cl⁻ M06-2X Energy= -
1625.08926680 Hartree

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 C,1.4189578537,1.9160567851,-1.0093555571
 C,0.716262592,2.9587503555,-0.2985991332
 C,-0.6649836467,2.9540644919,-0.319156525
 C,1.2040989792,-0.3666983704,-1.7971015398
 C,2.2741909382,-0.7160800038,-1.0093555571
 C,3.0421390438,0.2618777914,-0.2745192696
 C,2.615070091,1.5762608789,-0.2745192696
 C,0.0392903961,-1.2047389542,-1.8167452034
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 C,-2.21071492,-0.7183048193,-1.081703649
 C,-2.2672563617,-1.9704418595,-0.3615676428
 C,-1.1485772606,-2.7825006283,-0.3532046013
 C,-0.676341191,0.9977486034,-1.8167452034
 C,-1.3535735698,1.9179453818,-1.061798949
 C,-2.5647313554,1.5759735222,-0.3532046012
 C,-2.9924455924,0.2614611006,-0.3615676428
 C,-2.7285227545,2.62689706,0.6661054602
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 C,-3.3273231193,-1.7930054301,0.6448512105
 C,-0.66336993,-3.7289897994,0.6661054601
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 C,3.3560365836,-1.7954711931,0.7317115942
 C,3.7758715421,-0.5086619991,0.743866733
 C,2.7557602272,2.6309178058,0.7438667331
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 H,-3.6398424887,-2.5523368943,1.3495066307
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 H,3.652027918,-2.5567957545,1.4411183873
 H,4.460810884,-0.0801441651,1.4631776716
 H,3.5617642581,2.6868368388,1.4631776716
 H,1.451705816,4.215099366,1.4411183873
 H,-1.4443656316,4.2133401817,1.3989530891
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 H,3.1933564422,1.0375844034,-3.5076802681
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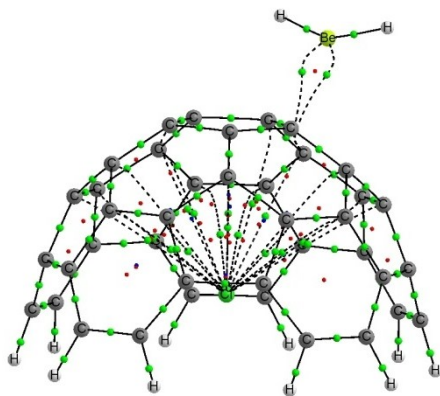
[66]BeH₂: C₃₀H₁₀:Cl⁻ M06-2X Energy= -
1625.09172038 Hartree

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 C,-0.0932011001,1.8850869632,-2.3272325186
 C,1.4872497413,0.4032293994,1.1426638367
 C,0.6858996516,0.6985753473,2.2136352907
 C,-0.1345937199,1.8876335634,2.2559942986
 C,-0.1903087892,2.7014192978,1.1404913199
 C,1.6033519606,-0.9544107348,0.6984869665
 C,0.9078490834,-1.9303948425,1.3617209892
 C,0.1444204088,-1.6465668052,2.5599494204
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 H,-1.4341966403,-2.8928862758,-3.599331328
 H,-1.3300835796,-4.4168735666,-1.489380479
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 Be,2.6183272167,3.2308055391,0.0025254837
 H,2.9562674773,3.4954488495,-1.2810359998
 H,2.9434095392,3.4500378475,1.2977869838
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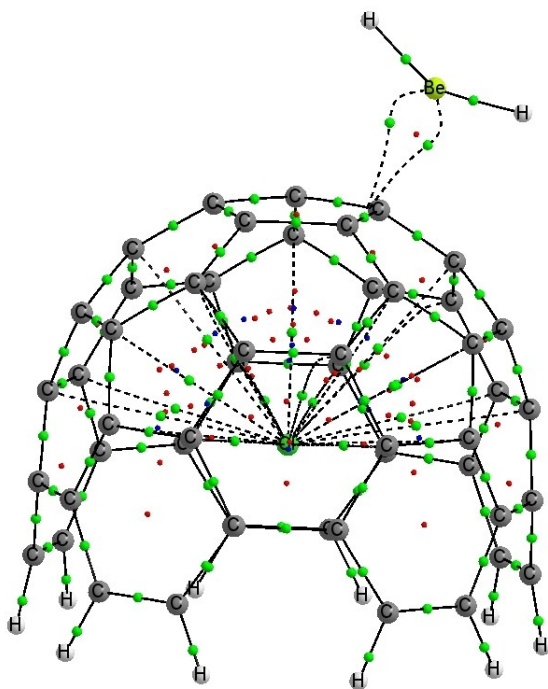
[65] BeH₂: C₄₀H₁₀:Cl⁻ M06-2X Energy= -2006.14571282 Hartree

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 C,-0.6991438618,2.9226616449,-1.0086482536
 C,1.1569693049,-0.3903374261,-2.5231179605
 C,2.264535816,-0.7405247733,-1.7744771466
 C,2.9968531951,0.2427517175,-1.0227402402
 C,2.5671910408,1.5651158517,-1.0227402402
 C,-0.0188968734,-1.2369529937,-2.5155001035
 C,-0.0107681529,-2.3961794785,-1.7709158758
 C,1.1522781523,-2.7754293884,-1.0086482537
 C,2.2821865416,-1.9631001254,-1.0155101144
 C,-1.1875141019,-0.3858467226,-2.511966299
 C,-2.2852225226,-0.7425138105,-1.7556917127
 C,-2.2880607934,-1.9604467841,-0.9879146123
 C,-1.1622062442,-2.7792958129,-0.9953744537
 C,-0.7423506212,0.9896086881,-2.5155001035
 C,-1.417150582,1.9322205553,-1.7709158758
 C,-2.5738736964,1.5653698492,-0.9953744537
 C,-3.0034017741,0.2411463679,-0.9879146123
 C,-2.6315825914,2.3498264238,0.1877148092
 C,-3.5062698766,-0.3493898449,0.2027518935
 C,-3.0419981114,-1.7782714082,0.2027518935
 C,-0.747801714,-3.4478549497,0.1877148091
 C,0.7537367216,-3.4472693453,0.1782737205
 C,3.0531904763,-1.7815814226,0.1633305253
 C,3.5168235234,-0.3511927105,0.159029179
 C,2.6387440959,2.3512578786,0.1590291791
 C,1.4228956897,3.2359499851,0.1633305253
 C,-1.4164682715,3.2319348106,0.1782737205
 C,-3.3146149501,1.8308741372,1.276401717
 C,-3.7517699385,0.4821588045,1.2840996324
 C,-2.7518397993,-2.5953097124,1.2840996324
 C,-1.6054190007,-3.4294900796,1.276401717
 C,1.6273209015,-3.4302363645,1.2537993898
 C,2.7755802277,-2.5975097238,1.2477679447
 C,3.7717872733,0.479090091,1.2371801955
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 C,0.7187136574,3.7328746354,1.2477679447
 C,-0.69971209,3.7316347387,1.2537993899
 H,-3.3245028019,2.3664488032,2.2206639161
 H,-4.0718335329,0.0638135835,2.2332788813
 H,-3.256673838,-2.4449899808,2.2332788813
 H,-1.2986155497,-3.868591019,2.2206639161
 H,1.3337114641,-3.8703502878,2.2018036981
 H,3.2912760288,-2.4481493406,2.1911599204
 H,4.1002680625,0.0604402652,2.1833804763
 H,3.3527124357,2.3611799028,2.1833804763
 H,1.2237121546,3.9151579347,2.1911599204
 H,-1.1959395885,3.9151150839,2.2018036981
 Be,1.8790988084,0.6105562162,-4.4615411373
 H,3.1439295365,1.0215246336,-4.2459824462
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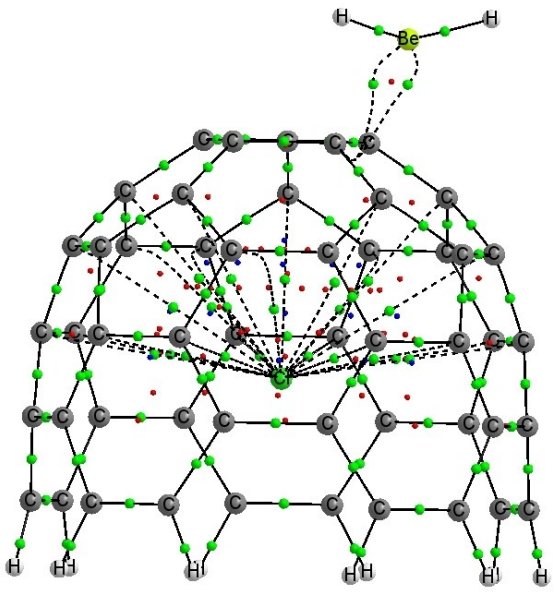
[66] BeH₂: C₄₀H₁₀:Cl⁻ M06-2X Energy= -2006.14525676 Hartree

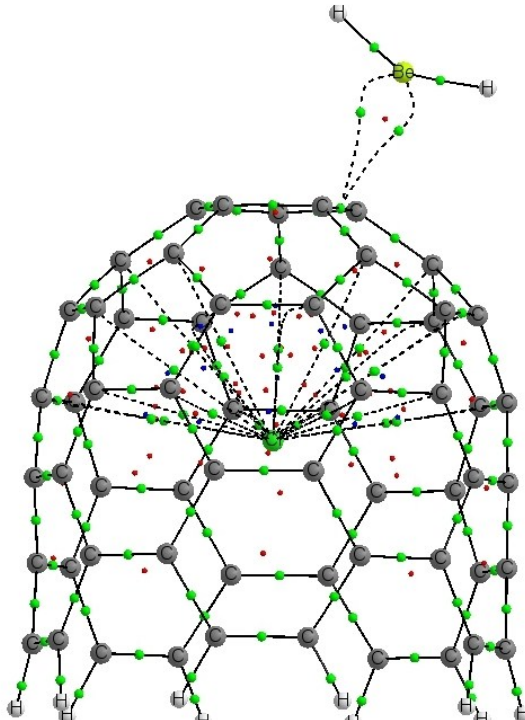
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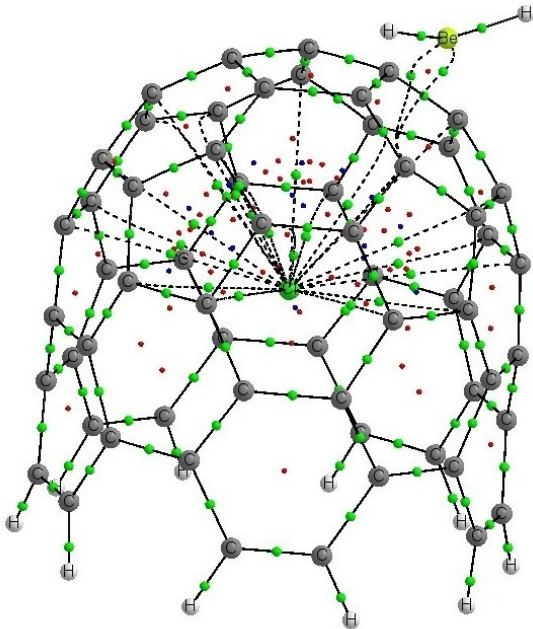


[65] BeH₂: C₅₀H₁₀:Cl⁻ M06-2X Energy= -2387.20051338 Hartree

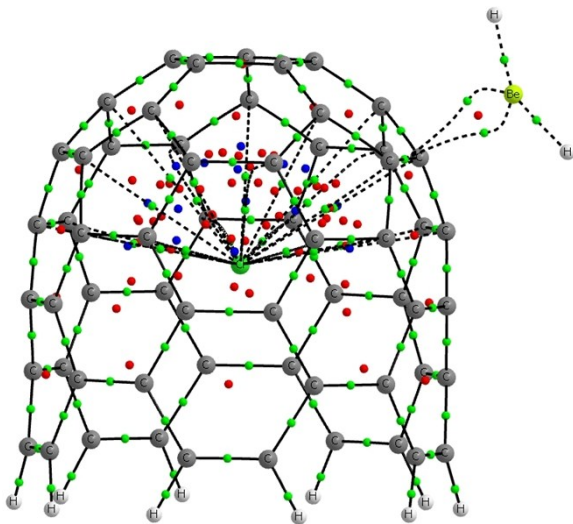
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	<p>H,1.1964493097,3.5366328832,3.2019528374 H,-1.1965755557,3.5362148575,3.1938095448 H,-3.0003784762,2.2374233211,3.1811800205 Be,1.188803648,1.6362757468,-4.8737859257 H,1.9678478547,2.7085566638,-4.6281635974 H,0.5968659498,0.8215292419,-5.7720570566 Cl,0.0145066921,0.0199671546,0.4276389422</p>
	<p>[66] BeH₂: C₅₀H₁₀:Cl M06-2X Energy= -2387.20058051 Hartree</p> <p>C,-0.0000000164,1.2405667079,-2.9217199134 C,-0.0000000229,2.4106489641,-2.1618582563 C,-1.1602027766,2.777689228,-1.3865184625 C,-2.2688551018,1.9668607457,-1.3917085294 C,1.1762304986,0.3926877601,-2.9290592001 C,2.2810856385,0.7556970242,-2.1744666646 C,2.2688550665,1.9668607784,-1.3917085414 C,1.1602027296,2.7776892448,-1.3865184686 C,0.7247044041,-0.9817255162,-2.9328910873 C,1.4094564201,-1.9245571942,-2.1795559208 C,2.5588314186,-1.538320052,-1.3976632255 C,2.9879075895,-0.2324299755,-1.3980663759 C,-0.7247044049,-0.9817255267,-2.9328910835 C,-1.4094564033,-1.9245572146,-2.1795559134 C,-0.6875504965,-2.897884285,-1.3999442977 C,0.6875505314,-2.8978842751,-1.3999443013 C,-1.1762305192,0.3926877431,-2.9290591939 C,-2.2810856604,0.7556969912,-2.1744666341 C,-2.9879075931,-0.2324300186,-1.3980663602 C,-2.5588314033,-1.538320089,-1.397663212 C,-3.4190710932,0.3648983098,-0.1583833327 C,-2.5567610054,-2.2786479206,-0.1602341583 C,-1.3902933204,-3.1242156588,-0.1605908293 C,1.3902933651,-3.1242156387,-0.1605908366 C,2.5567610379,-2.2786478836,-0.1602341717 C,3.4190710875,0.3648983592,-0.1583833507 C,2.9724478257,1.734703501,-0.154841204 C,0.7204510449,3.3687157371,-0.1494233148 C,-0.720451094,3.3687157267,-0.149423311 C,-2.9724478511,1.734703458,-0.1548411884 C,-3.5067806897,-0.3552085608,1.0289375777 C,-3.0521836058,-1.7492539402,1.028071783 C,-0.7332713175,-3.4294559318,1.0279104983 C,0.7332713728,-3.4294559212,1.0279104945 C,3.0521836369,-1.7492538961,1.028071767 C,3.5067807006,-0.3552085102,1.0289375593 C,2.6206147605,2.366433641,1.0341213745 C,1.4325949022,3.226296526,1.0383103841 C,-1.4325949429,3.2262965053,1.0383103917 C,-2.6206147889,2.3664336032,1.0341213883 C,-3.5341695327,0.4377286602,2.2272485791 C,-2.6037950074,-2.4036717427,2.2257569647 C,-1.4956253399,-3.2069267253,2.2254516382 C,1.4956253983,-3.2069267037,2.2254516303 C,2.6037950543,-2.4036717051,2.225756951 C,3.5341695385,0.4377287113,2.2272485605 C,3.1112737774,1.739174778,2.2299811327 C,0.6847305343,3.4849078006,2.2360682785 C,-0.6847305725,3.4849077907,2.2360682821 C,-3.1112737904,1.739174733,2.229981149</p>

	<p>H,-3.7532267282,-0.0319463835,3.1800418659 H,-3.0493084109,-2.144754525,3.1802733644 H,-1.1120127384,-3.5496649361,3.1802347966 H,1.1120128068,-3.54966492,3.1802347908 H,3.049308459,-2.1447544809,3.1802733484 H,3.7532267458,-0.0319463293,3.1800418462 H,3.0103585488,2.2452359739,3.1838168857 H,1.1957996826,3.5296134694,3.1915020155 H,-1.1957997165,3.5296134522,3.1915020217 H,-3.0103585641,2.2452359304,3.1838169016 Be,-0.0000000331,3.0000574525,-4.4290889126 H,-1.298576973,3.1964028246,-4.7384656178 H,1.2985769024,3.1964028434,-4.7384656246 Cl,0.000000013,0.0096293659,0.4261867364</p>
	<p>[65] BeH₂: C₆₀H₁₀:Cl⁻ M06-2X Energy= -2768.24323497 Hartree</p> <p>C,3.2985051411,1.2504765788,-0.7285681987 C,3.2530135602,0.0378358043,-1.4090728847 C,3.209328412,-1.2074794201,-0.6862288877 C,3.209328412,-1.2074794201,0.6862288877 C,2.4738574835,2.3577407489,-1.1704818397 C,1.6586057629,2.1973900388,-2.2813766775 C,1.6181481433,0.9319378423,-2.9758817849 C,2.3996518663,-0.1168957456,-2.5595062729 C,1.9705847423,3.0405947447,0. C,0.670205261,3.530460463,0. C,-0.172696687,3.3500969783,-1.1565340705 C,0.3082109209,2.7002317291,-2.2666346583 C,2.4738574835,2.3577407489,1.1704818397 C,1.6586057629,2.1973900388,2.2813766775 C,0.3082109209,2.7002317291,2.2666346583 C,-0.172696687,3.3500969783,1.1565340705 C,3.2985051411,1.2504765788,0.7285681987 C,3.2530135602,0.0378358043,1.4090728847 C,2.3996518663,-0.1168957456,2.5595062729 C,1.6181481433,0.9319378423,2.9758817849 C,1.8425180275,-1.4536598141,2.539811726 C,0.2572871869,0.678006186,3.3999984005 C,-0.5447039965,1.7573074343,2.9616838417 C,-1.5223769304,3.0778872608,0.7072109155 C,-1.5223769304,3.0778872608,-0.7072109155 C,-0.5447039965,1.7573074343,-2.9616838417 C,0.2572871869,0.678006186,-3.3999984005 C,1.8425180275,-1.4536598141,-2.539811726 C,2.3384138617,-2.1221472031,-1.3960258218 C,2.3384138617,-2.1221472031,1.3960258218 C,0.550793908,-1.7303862225,3.0146919831 C,-0.2760297532,-0.6192818984,3.4626393335 C,-1.8799709397,1.5391293213,2.5888840232 C,-2.3899538859,2.2285767648,1.4132291879 C,-2.3899538859,2.2285767648,-1.4132291879 C,-1.8799709397,1.5391293213,-2.5888840232 C,-0.2760297532,-0.6192818984,-3.4626393335 C,0.550793908,-1.7303862225,-3.0146919831 C,1.5393590728,-3.0638375527,-0.7279393659 C,1.5393590728,-3.0638375527,0.7279393659 C,-0.0874968934,-2.9200173682,2.5629473484 C,-1.6925572063,-0.761373189,3.434140514 C,-2.4976767455,0.3214699663,2.9946438316</p>

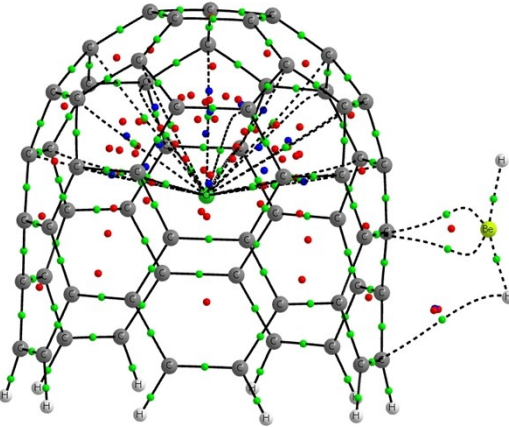
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	<p>[66] BeH₂: C₆₀H₁₀·Cl⁻ M06-2X Energy= -2768.24434546 Hartree</p> <p>C,-1.1759179035,-0.337455302,-3.5725856646 C,-2.2833015418,-0.7096248916,-2.8244734354 C,-2.2678299926,-1.9279886343,-2.0514181476 C,-1.1598929706,-2.7363512582,-2.0553969394 C,-0.724784773,1.0376370054,-3.5613889889 C,-1.4105754778,1.9740202237,-2.8014353412 C,-2.5569406096,1.5756393218,-2.0195158115 C,-2.9849701061,0.2712999628,-2.0331526585 C,0.724784773,1.0376370054,-3.5613889889 C,1.4105754778,1.9740202237,-2.8014353412 C,0.6864718882,2.9366395468,-2.0086274112 C,-0.6864718882,2.9366395468,-2.0086274112 C,1.1759179035,-0.337455302,-3.5725856646 C,2.2833015418,-0.7096248916,-2.8244734354 C,2.9849701061,0.2712999628,-2.0331526585 C,2.5569406096,1.5756393218,-2.0195158115 C,0,-1.1822894142,-3.571255671 C,0,-2.3681383582,-2.8348348052 C,1.1598929706,-2.7363512582,-2.0553969394 C,2.2678299926,-1.9279886343,-2.0514181476 C,0.7074858744,-3.3344778036,-0.8200934772 C,2.9663981178,-1.6950602552,-0.8045376029 C,3.4017965893,-0.3496661506,-0.7925506347 C,2.5391165073,2.3040158237,-0.7690385904 C,1.3946501115,3.1353679576,-0.7610005724 C,-1.3946501115,3.1353679576,-0.7610005724</p>

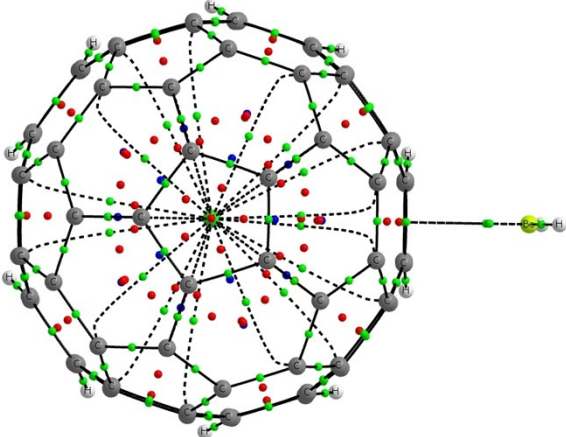
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H,-1.2043394957,3.4704190842,3.8275759124
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H,-3.0348506638,-2.1614758018,3.7768932598
H,-1.0878847086,-3.5814163591,3.7611001437
Be,0,-3.0317382878,-5.0406807599
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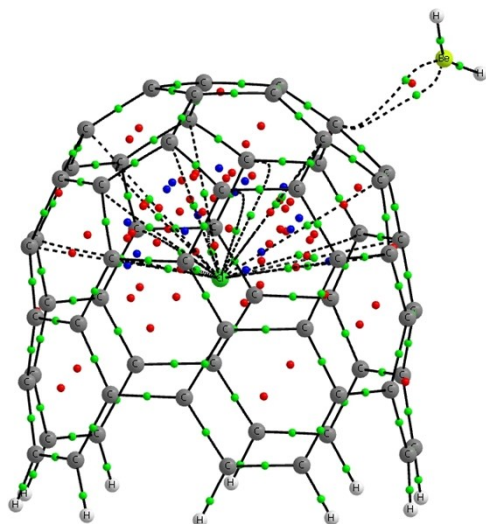
A BeH₂: C₆₀H₁₀:Cl⁻ M06-2X = -2768.24448104 Hartree

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 C,3.3088213407,0.887734394,0.6906990677
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 C,-0.9805008569,-1.511792698,-3.435329741
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 C,2.3548149222,-2.6603620477,1.4136476754
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	<p>C,0.5814725729,-3.3375529511,-3.0398688975 C,2.2130722148,-3.8995935111,-0.6763846351 C,2.2130722148,-3.8995935111,0.6763846351 H,0.7753970934,-4.4010010049,2.9590881038 H,-1.3911781983,-3.6561643443,3.7034126735 H,-3.3540106819,-2.9786466758,3.0386152989 H,-4.6934871463,-2.514973219,1.0899571418 H,-4.6934871463,-2.514973219,-1.0899571418 H,-3.3540106819,-2.9786466758,-3.0386152989 H,-1.3911781983,-3.6561643443,-3.7034126735 H,0.7753970934,-4.4010010049,-2.9590881038 H,1.9954820041,-4.8207140509,-1.2048379816 H,1.9954820041,-4.8207140509,1.2048379816 Be,5.4922923235,1.3375146183,0. H,6.1133101933,0.1402454667,0. H,5.5803811191,2.6835073693,0. Cl,-0.0294303458,0.0977271244,0.</p>
	<p>B BeH₂:C₆₀H₁₀:Cl⁻ M06-2X =-2768.24428472 Hartree</p> <p>C,3.5227144837,-0.7476893156,-0.7242666533 C,2.8174463143,-1.7264983824,-1.4113018457 C,2.0800112646,-2.7307990197,-0.6858394048 C,2.0800112647,-2.7307990206,0.6858394011 C,3.4571213629,0.6283111115,-1.1714872993 C,2.6898809364,0.9532961429,-2.2820819086 C,1.9538095404,-0.0709945201,-2.9818719049 C,2.0160965732,-1.3748741794,-2.558489196 C,3.4180549392,1.4785009394,0.0000000009 C,2.6128286089,2.6098710565,0.0000000017 C,1.8114795025,2.930401584,-1.1561405194 C,1.849965953,2.1256878461,-2.2673719929 C,3.4571213629,0.628311111,1.1714873 C,2.6898809365,0.9532961399,2.2820819098 C,1.8499659531,2.1256878431,2.2673719956 C,1.8114795025,2.9304015825,1.1561405232 C,3.5227144837,-0.7476893165,0.7242666522 C,2.8174463143,-1.7264983843,1.4113018434 C,2.0160965733,-1.3748741827,2.5584891942 C,1.9538095405,-0.070994524,2.9818719047 C,0.8063298665,-2.1705016246,2.5411072884 C,0.6807573045,0.4781661869,3.4010503621 C,0.6167634256,1.821132744,2.9629431458 C,0.5396913244,3.4573589977,0.7070016781 C,0.5396913244,3.4573589987,-0.7070016736 C,0.6167634255,1.8211327479,-2.9629431434 C,0.6807573044,0.4781661913,-3.4010503615 C,0.8063298665,-2.1705016213,-2.5411072912 C,0.8459627116,-2.9956157374,-1.394368648 C,0.8459627117,-2.9956157392,1.3943686441 C,-0.4222394486,-1.6802163251,3.0138815423 C,-0.487329683,-0.2989863833,3.4678476126 C,-0.614702487,2.3838480228,2.5892891578 C,-0.6547220931,3.2379438627,1.4123312372 C,-0.6547220932,3.2379438646,-1.4123312329 C,-0.614702487,2.3838480262,-2.5892891547 C,-0.4873296831,-0.2989863787,-3.467847613 C,-0.4222394486,-1.6802163211,-3.0138815445 C,-0.3463741494,-3.3430039442,-0.7332457113 C,-0.3463741494,-3.3430039451,0.733245707 C,-1.6170704433,-2.3127705549,2.566524514</p>

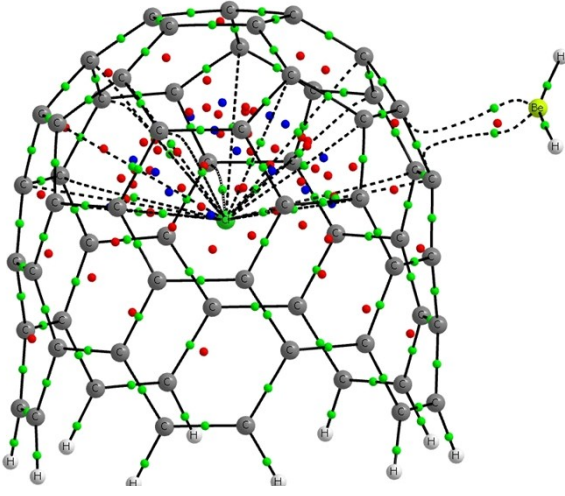
	<p>C,-1.7417806607,0.3726250547,3.438530213 C,-1.8061112011,1.7203217841,2.9983884068 C,-1.8843716609,3.3807066403,0.7096875616 C,-1.8843716609,3.3807066412,-0.7096875571 C,-1.8061112011,1.720321788,-2.9983884045 C,-1.7417806608,0.3726250591,-3.4385302125 C,-1.6170704434,-2.3127705516,-2.566524517 C,-1.5825409197,-3.1402529129,-1.4154847077 C,-1.5825409197,-3.1402529148,1.4154847036 C,-2.8623094106,-1.7539561265,3.0535305173 C,-2.9215729233,-0.4686180656,3.4697729796 C,-3.0537197351,2.3102635058,2.5573003942 C,-3.0909105671,3.1048316989,1.4631825591 C,-3.0909105672,3.1048317008,-1.4631825549 C,-3.0537197352,2.3102635091,-2.5573003911 C,-2.9215729234,-0.468618061,-3.4697729801 C,-2.8623094107,-1.7539561225,-3.0535305195 C,-2.7846188696,-3.4574867268,-0.6759908037 C,-2.7846188696,-3.4574867277,0.6759907992 H,-3.7772202465,-2.3311157359,2.9837903384 H,-3.8836818068,-0.0386288341,3.7242923991 H,-3.9837879115,2.027408942,3.0370593493 H,-4.0502945287,3.4436622468,1.0886077712 H,-4.0502945287,3.4436622482,-1.0886077666 H,-3.9837879116,2.027408946,-3.0370593465 H,-3.8836818069,-0.0386288293,-3.724292399 H,-3.7772202466,-2.331115732,-2.9837903413 H,-3.7212658205,-3.5940996265,-1.2036496838 H,-3.7212658204,-3.5940996281,1.2036496792 Be,-0.0231176256,-5.5777425879,-0.0000000036 H,-1.271112752,-6.0840102866,-0.000000004 H,1.3108479701,-5.7388253976,-0.0000000038 Cl,0.046237273,0.0765625574,0.</p>
	<p>C BeH₂:C₆₀H₁₀:Cl⁻ M06-2X = -2768.24704941</p> <p>C,3.5858002586,-1.1865916545,-0.7238706127 C,2.8937306297,-2.1747697118,-1.4108215778 C,2.168387328,-3.1897356891,-0.6862750309 C,2.168387328,-3.1897356891,0.6862750309 C,3.5032622109,0.1882775937,-1.1711887871 C,2.7349811104,0.5055425567,-2.2823194405 C,2.0087903006,-0.5277326974,-2.9795006165 C,2.0883492367,-1.8314806802,-2.5574911476 C,3.4536501539,1.0394187915,0. C,2.6347882792,2.1599965318,0. C,1.8314195614,2.4735307364,-1.1567105454 C,1.8800783893,1.6677573184,-2.2666803259 C,3.5032622109,0.1882775937,1.1711887871 C,2.7349811104,0.5055425568,2.2823194406 C,1.8800783893,1.6677573184,2.2666803259 C,1.8314195614,2.4735307364,1.1567105454 C,3.5858002586,-1.1865916545,0.7238706127 C,2.8937306297,-2.1747697118,1.4108215778 C,2.0883492367,-1.8314806802,2.5574911476 C,2.0087903005,-0.5277326974,2.9795006165 C,0.8860476697,-2.6379239945,2.5345814854 C,0.7309970477,0.0071230516,3.4023988895 C,0.6512808888,1.3488507499,2.9635336045 C,0.552654725,2.9844322008,0.7070358965 C,0.552654725,2.9844322008,-0.7070358965</p>

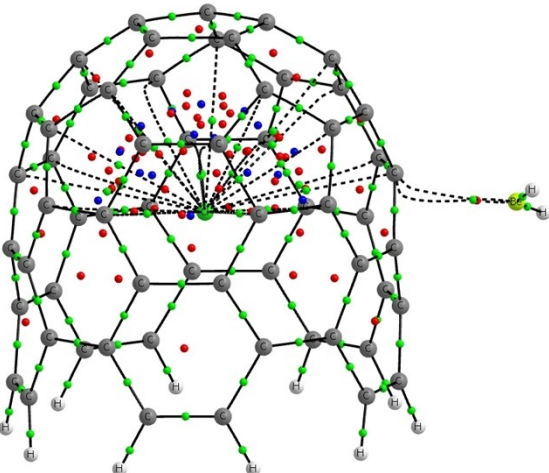
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C,-0.6389583133,2.7507417135,-1.412859835
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C,-0.3460481473,-2.1643512154,-3.0170496164
C,-0.2475014355,-3.8216179689,-0.7268757961
C,-0.2475014355,-3.8216179689,0.7268757961
C,-1.5310070134,-2.8114933285,2.5716272754
C,-1.6894022397,-0.1268862623,3.4435621763
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C,-2.857541057,-0.983220604,3.4749368825
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C,-2.6792271102,-3.9604772675,0.683298778
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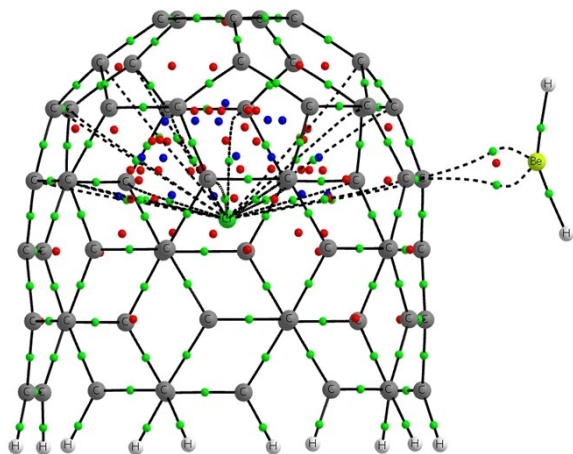
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 C,2.9102400784,0.1285195108,-2.2157059802
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 C,1.0440693032,-2.8563276711,-2.1597942612
 C,2.1617337213,-2.0541204889,-2.1784653525
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 C,2.875340655,-1.8106403759,-0.9440238309
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 C,-0.8060166446,-3.4192349411,1.5249540637
 C,1.3790640981,-3.2095306481,2.724684059
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 C,-3.5001438826,0.4299564854,2.7173420544

	<p>C,-2.6306154524,-2.3655332756,2.7449422728 C,-1.5475610966,-3.1765981531,2.7460691153 H,1.0073590169,-3.5778868911,3.6741347167 H,2.9719018206,-2.1826770455,3.6437937054 H,3.6717077256,-0.12042685,3.613426881 H,2.9583740608,2.1817826613,3.5900960987 H,1.2139247388,3.4826370647,3.5865858235 H,-1.1955261291,3.5086191388,3.6056836341 H,-2.9732897237,2.2511628504,3.6345771885 H,-3.7478741562,-0.0299568306,3.6671978853 H,-3.0997074489,-2.1090024237,3.6881346609 H,-1.1715039078,-3.5544699669,3.6899866554 Be,0.9454284642,-4.1170678517,-4.1391753143 H,1.7552232493,-3.4788173487,-5.0065441106 H,0.3196255101,-5.2487976992,-3.7544703541 Cl,-0.0642417021,-0.0684365411,-0.3456564749</p>
	<p>E BeH₂:C₆₀H₁₀:Cl M06-2X = -2768.24515208 C,-1.310555815,-0.4184815854,-3.8513255137 C,-2.4217409567,-0.7703757459,-3.0983759835 C,-2.4198548293,-1.992216952,-2.3321721461 C,-1.3235394466,-2.8222799308,-2.358267731 C,-0.8376920467,0.9518500758,-3.836629046 C,-1.4984711652,1.8972122476,-3.0660835002 C,-2.644728873,1.5161897267,-2.2747561725 C,-3.094620709,0.2196053319,-2.291772974 C,0.609498392,0.925827611,-3.851907223 C,1.3219499627,1.8450628111,-3.095457883 C,0.6251196008,2.8170172169,-2.2894211976 C,-0.7477433381,2.8417618112,-2.2749026077 C,1.0309409506,-0.4597312732,-3.872525809 C,2.1498789767,-0.8496885641,-3.1498768807 C,2.8759199995,0.1135130738,-2.3579434825 C,2.4724601507,1.42440478,-2.3308062914 C,-0.156248358,-1.2904221471,-3.8799423136 C,-0.172188868,-2.4675043301,-3.1467461823 C,0.9907052203,-2.859035627,-2.3862156738 C,2.1156271627,-2.0652342282,-2.37653383 C,0.5454873059,-3.4611925057,-1.1380815354 C,2.8371866027,-1.8604662743,-1.141020124 C,3.2998218226,-0.5230071448,-1.1267282425 C,2.4805198882,2.143639149,-1.0745356687 C,1.3504313872,2.9941297623,-1.0487302119 C,-1.4391759824,3.0455005411,-1.0192614168 C,-2.5989505836,2.2350249974,-1.0195510717 C,-3.5114842901,-0.400292685,-1.0514570587 C,-3.0982500402,-1.7541295228,-1.0774907423 C,-0.8727081032,-3.4285403472,-1.1273687589 C,1.26910998,-3.3164854042,0.0615393589 C,2.4642583955,-2.4930656703,0.0568547698 C,3.383896765,0.1777180992,0.0869487205 C,2.9585766488,1.5692853414,0.1144910534 C,0.7010064891,3.2689512403,0.16555568 C,-0.7539023281,3.2960255729,0.1805848424 C,-3.0723703784,1.6785634681,0.1795714865 C,-3.5482411985,0.3038808263,0.1624918576 C,-2.7217677849,-2.3989922349,0.1116795272 C,-1.5595555996,-3.2724977948,0.0856226665 C,0.5758839277,-3.5264016193,1.2852540424 C,2.8958694433,-1.9133812661,1.2835110315 C,3.357549338,-0.572295381,1.2978162909</p>

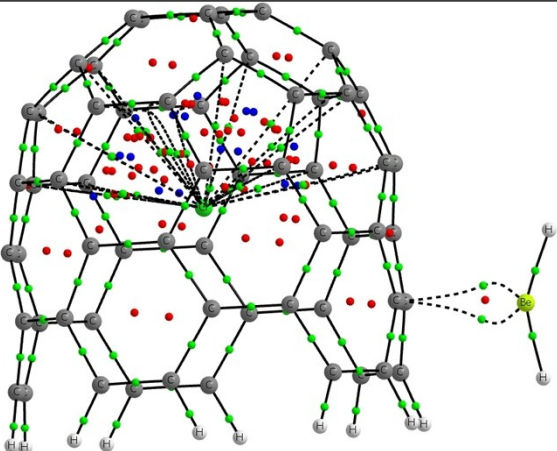
	<p>C,2.527686192,2.131020633,1.349608595 C,1.3957719237,2.9860862541,1.3752997186 C,-1.4316205019,3.0358133329,1.4051397662 C,-2.5965713713,2.2252740834,1.4046511543 C,-3.5196333179,-0.4470753241,1.372447999 C,-3.1059818899,-1.8039757637,1.3462175622 C,-0.8427994662,-3.4988449962,1.2961585617 C,1.3472610364,-3.3449885699,2.4984323382 C,2.4580183423,-2.5733662902,2.4971765546 C,3.409225654,0.1913856216,2.5282068922 C,3.0107060976,1.4838430421,2.5528691279 C,0.675692291,3.2477096619,2.6053742696 C,-0.6769475419,3.2713632123,2.6196888595 C,-3.0782871949,1.5967023857,2.6180046838 C,-3.520676735,0.3179898692,2.6027242124 C,-2.6623547589,-2.479399293,2.5487180736 C,-1.5814121426,-3.2928375738,2.5253995046 H,0.9784632854,-3.7420679553,3.4372700062 H,2.9574371632,-2.3631208387,3.4359804218 H,3.6600628287,-0.303690173,3.4593326915 H,2.9503459848,2.0005440421,3.5039630962 H,1.2155785055,3.3135070726,3.5432613032 H,-1.1937828812,3.356888745,3.5687404982 H,-2.9820279958,2.111064524,3.5675315896 H,-3.771080969,-0.1659257466,3.5399671613 H,-3.1284664356,-2.249159713,3.5001458063 H,-1.2022073224,-3.6975470857,3.4566428623 Be,1.5893039406,-5.0746648038,-2.4069575522 H,2.8384062575,-5.1492034379,-1.9053970782 H,0.6035748496,-5.6358406146,-3.1380347287 Cl,-0.0923741732,-0.1075086602,-0.4957499259</p>
	<p>F BeH₂·C₆₀H₁₀·Cl·M06-2X = -2768.24594994</p> <p>C,-1.4977103048,-0.1922290042,-4.8573379563 C,-2.6096137271,-0.5597694276,-4.1111248899 C,-2.6005768164,-1.7873854974,-3.3548796295 C,-1.4979304708,-2.6075383564,-3.38401942 C,-1.0374309631,1.181569304,-4.8270320062 C,-1.7105271543,2.1141068234,-4.0510713676 C,-2.8571340501,1.7170343595,-3.2691612468 C,-3.2951285784,0.4170669073,-3.2999917619 C,0.4108446851,1.168418207,-4.836813832 C,1.1096621357,2.0877698009,-4.0668634639 C,0.3988661459,3.0461404332,-3.2559860306 C,-0.9737373692,3.0595902483,-3.2485481572 C,0.8450489821,-0.2128309022,-4.8722611079 C,1.9578007417,-0.6022264434,-4.1385745139 C,2.6700731085,0.3611401939,-3.3338786957 C,2.2576546335,1.669892591,-3.299370972 C,-0.3345961557,-1.0525706824,-4.8866648171 C,-0.3411454721,-2.2387934834,-4.163466653 C,0.8168658149,-2.6253420778,-3.3993865208 C,1.9344416741,-1.8300533481,-3.3834251584 C,0.3677482789,-3.2438604748,-2.1656289913 C,2.6421707739,-1.6205020356,-2.1363714422 C,3.0922957245,-0.2798491577,-2.1060566943 C,2.252511062,2.3788783884,-2.0366467617 C,1.1159947053,3.2207653386,-2.0103549146 C,-1.6731261396,3.2458390502,-1.9941224755 C,-2.8257541307,2.4258510865,-2.007098938</p>

C,-3.712260203,-0.2174042293,-2.0664337571
C,-3.2910631245,-1.5673254267,-2.1020340584
C,-1.0517269817,-3.2170069666,-2.1534499564
C,1.0821804975,-3.1008352764,-0.9558275968
C,2.2731711567,-2.2636268529,-0.9460430473
C,3.165466785,0.4117724073,-0.8857971077
C,2.7301623197,1.7999373751,-0.850017156
C,0.4583160796,3.480945237,-0.79701389
C,-0.9966776211,3.4941763702,-0.788630061
C,-3.2979510601,1.8538577227,-0.8145891624
C,-3.7605387076,0.4751655222,-0.8458608246
C,-2.9179566964,-2.2198146984,-0.916095551
C,-1.7467862452,-3.0807701192,-0.943754153
C,0.3824656668,-3.3327627561,0.2640657543
C,2.6870357665,-1.6911500435,0.2877213604
C,3.139153272,-0.3467903935,0.3185600676
C,2.2893339767,2.3489839207,0.3873825549
C,1.1496948826,3.1936117979,0.413824196
C,-1.6781806055,3.2182438237,0.4309798175
C,-2.8332496519,2.3948624918,0.4178510631
C,-3.7340707051,-0.2852407817,0.3579639558
C,-3.3101002864,-1.6390682624,0.3223561113
C,-1.0367041012,-3.3187588004,0.2666672167
C,1.1490062239,-3.1562856055,1.4817148448
C,2.2507155831,-2.3724302276,1.4913204761
C,3.178625706,0.4071067889,1.5551781985
C,2.7727633006,1.697169327,1.5877461357
C,0.4217486355,3.4397465997,1.6425418777
C,-0.9307878253,3.4518727558,1.6507902977
C,-3.3128245313,1.7501949002,1.6235928069
C,-3.7457796739,0.4689809948,1.59514646
C,-2.864733822,-2.3209110715,1.5204306764
C,-1.7804147325,-3.1298247477,1.4947210145
H,0.782656162,-3.5718571699,2.4131547933
H,2.7486268195,-2.1733217769,2.4334859241
H,3.4302290398,-0.0922313773,2.4840184214
H,2.7062813075,2.2062606439,2.5425883392
H,0.9571227032,3.5045114843,2.5830247568
H,-1.4537387855,3.5257826989,2.5975700535
H,-3.2231031794,2.2561978218,2.5781631461
H,-3.99501917,-0.0260492427,2.5269783009
H,-3.3345781691,-2.0998355058,2.4722840705
H,-1.4024659209,-3.5421564275,2.4228356611
Be,1.1846332938,-5.3052376002,-1.7254380989
H,2.4484725865,-5.3659810429,-2.1985122606
H,0.1094611097,-5.9850347182,-1.2719974961
Cl,-0.3044616486,0.090527066,-1.4609679368



I BeH₂:C₆₀H₁₀:Cl⁻ M06-2X =-2768.24693499 Hartre

C,3.4524370757,-0.6797446197,-1.1727708578
 C,2.6663004537,-0.9538809099,-2.2840572339
 C,1.7517363683,-2.0685658637,-2.2683371098
 C,1.6656798953,-2.8696901211,-1.1565430701
 C,3.607185814,0.6901306102,-0.7254809845
 C,2.9658691408,1.7118703483,-1.4109376042
 C,2.1414442048,1.4129845637,-2.5578755415
 C,1.9970710892,0.1163993637,-2.9830732209
 C,3.6075338358,0.6900465615,0.722634272
 C,2.9668203212,1.7117366481,1.4087068484
 C,2.2958547552,2.7639643833,0.6855175797
 C,2.2953865431,2.7640148142,-0.6871651787
 C,3.4531216737,-0.6798229533,1.1699147327
 C,2.6678378267,-0.9540393072,2.2817635016
 C,1.9991474041,0.1161545381,2.9814125058
 C,2.1432296342,1.4127692374,2.5562093695
 C,3.3596911395,-1.5243157334,-0.0014176199
 C,2.4829471178,-2.603241451,-0.0011475706
 C,1.6664452078,-2.8696626268,1.1547658458
 C,1.7532752511,-2.0687081695,2.2665951917
 C,0.360463232,-3.3125064248,0.7118163378
 C,0.5426205756,-1.6843233716,2.9616876213
 C,0.6930690116,-0.3490665437,3.4009356359
 C,0.9888357906,2.2857962704,2.5379581765
 C,1.0818321414,3.1118317328,1.3938102296
 C,1.0808429719,3.1119119285,-1.3945387642
 C,0.9870381968,2.2859823745,-2.5386891471
 C,0.6906802769,-0.3487899681,-3.4016601831
 C,0.5405602993,-1.6840902809,-2.962494338
 C,0.3599689368,-3.3125007364,-0.7127009306
 C,-0.821628982,-3.009742025,1.4147454336
 C,-0.7241637564,-2.1674719941,2.5930513531
 C,-0.422323636,0.5028746545,3.4637586636
 C,-0.2677215133,1.8780991507,3.0144933166
 C,-0.0819126858,3.5296118173,0.7277404076
 C,-0.0824278845,3.52965356,-0.7276098154
 C,-0.2698614003,1.878325965,-3.0143340198
 C,-0.4247725369,0.5031540031,-3.4636029445
 C,-0.7259821425,-2.1672788233,-2.5930298028
 C,-0.822621697,-3.0096672189,-1.4147435619
 C,-2.0543624273,-3.0760446534,0.7104807605
 C,-1.8699166336,-1.4270078137,2.9990738332
 C,-1.7180598177,-0.0854980843,3.4367229275
 C,-1.4166837333,2.5874926328,2.5636533746
 C,-1.3233967409,3.4164909265,1.4150759042
 C,-1.3244041157,3.4165798492,-1.4140626472
 C,-1.41851001,2.5876916118,-2.5626403584
 C,-1.7204812657,-0.0852052715,-3.4357671619
 C,-1.8720188445,-1.4267732428,-2.9981576301
 C,-2.0548591019,-3.0760008251,-0.7095991963
 C,-3.2411167647,-2.7260772894,1.462788303
 C,-3.1518881553,-1.9341045861,2.5558111682
 C,-2.8404867065,0.8297890376,3.4630952527
 C,-2.6961765327,2.1086845756,3.0455545694
 C,-2.5035181944,3.8195025225,0.6775132487
 C,-2.5040003048,3.8195445994,-0.6756360617
 C,-2.6983273986,2.1089417007,-3.0437348586
 C,-2.8429214114,0.8300932361,-3.4613192948

	<p>C,-3.1536757941,-1.933909633,-2.5540559393 C,-3.2421368307,-2.7259754024,-1.4610365855 H,-4.2185714958,-3.0077307656,1.0892577059 H,-4.0620121179,-1.592589673,3.0357208051 H,-3.8297759024,0.4636508288,3.7129145002 H,-3.5733201345,2.7415499907,2.9706455706 H,-3.4298479567,4.0160862947,1.2053341636 H,-3.430705784,4.0161477082,-1.2027907341 H,-3.5754133923,2.7418145857,-2.9681957904 H,-3.8323696629,0.4639929371,-3.7105603943 H,-4.0641394958,-1.5923190441,-3.0332641574 H,-4.2193351139,-3.0076089171,-1.0868221452 Be,0.3948164686,-5.5043220629,-0.0001239218 H,1.6964583872,-5.8611724146,-0.0005096394 H,-0.9008037452,-5.8851714176,-0.0005397082 Cl,0.063632925,0.0683980229,-0.0001333895</p>
	<p>J BeH₂:C₆₀H₁₀:Cl⁻ M06-2X ==-2768.24788381 Hartree</p> <p>C,3.9815481524,-1.2047200594,-1.1716678556 C,3.1986853952,-1.476802332,-2.2844328141 C,2.2783171188,-2.5882552493,-2.2663743249 C,2.1865821047,-3.3913466263,-1.1570912761 C,4.1409481474,0.1636248774,-0.7239909454 C,3.5064037126,1.1886992481,-1.4109843997 C,2.6822916967,0.8922824798,-2.5582443948 C,2.5331443037,-0.4041421162,-2.9830057301 C,4.1409481474,0.1636248774,0.7239909454 C,3.5064037126,1.1886992481,1.4109843997 C,2.8393499409,2.2425140408,0.6865005895 C,2.8393499409,2.2425140408,-0.6865005895 C,3.9815481524,-1.2047200594,1.1716678556 C,3.1986853952,-1.476802332,2.2844328141 C,2.5331443037,-0.4041421162,2.9830057301 C,2.6822916967,0.8922824798,2.5582443948 C,3.8839115699,-2.0509264102,0. C,3.0059190085,-3.1252968457,0. C,2.1865821047,-3.3913466263,1.1570912761 C,2.2783171188,-2.5882552493,2.2663743249 C,0.8807891402,-3.8237476642,0.7072066579 C,1.0699313551,-2.2014214362,2.9643351863 C,1.2244780634,-0.8652322616,3.4003422981 C,1.5299966046,1.7689424201,2.5386658433 C,1.6259169261,2.5939658277,1.3941052874 C,1.6259169261,2.5939658277,-1.3941052874 C,1.5299966046,1.7689424201,-2.5386658433 C,1.2244780634,-0.8652322616,-3.4003422981 C,1.0699313551,-2.2014214362,-2.9643351863 C,0.8807891402,-3.8237476642,-0.7072066579 C,-0.2932266577,-3.5266448924,1.4151453919 C,-0.1971144545,-2.6797561676,2.5928516922 C,0.1120227525,-0.0094528981,3.4629787948 C,0.2717513804,1.3652813136,3.0143652753 C,0.4634056562,3.0152033525,0.7277139514 C,0.4634056562,3.0152033525,-0.7277139514 C,0.2717513804,1.3652813136,-3.0143652753 C,0.1120227525,-0.0094528981,-3.4629787948 C,-0.1971144545,-2.6797561676,-2.5928516922 C,-0.2932266577,-3.5266448924,-1.4151453919 C,-1.5355706948,-3.5930379124,0.7156764511 C,-1.3402921357,-1.9347066871,2.9962363542</p>

C,-1.1856259971,-0.594486756,3.4360367146
C,-0.8749222999,2.0771442855,2.5625667425
C,-0.7786978031,2.9060645642,1.4144001998
C,-0.7786978031,2.9060645642,-1.4144001998
C,-0.8749222999,2.0771442855,-2.5625667425
C,-1.1856259971,-0.594486756,-3.4360367146
C,-1.3402921357,-1.9347066871,-2.9962363542
C,-1.5355706948,-3.5930379124,-0.7156764511
C,-2.7243173813,-3.2362628747,1.4694965439
C,-2.6253628414,-2.4417262376,2.5589530256
C,-2.3058140968,0.3239163523,3.4606379757
C,-2.1565684987,1.6021008646,3.0429472061
C,-1.957834166,3.3115579252,0.6765644592
C,-1.957834166,3.3115579252,-0.6765644592
C,-2.1565684987,1.6021008646,-3.0429472061
C,-2.3058140968,0.3239163523,-3.4606379757
C,-2.6253628414,-2.4417262376,-2.5589530256
C,-2.7243173813,-3.2362628747,-1.4694965439
H,-3.698865653,-3.5305936098,1.1002926026
H,-3.5331196288,-2.0971421746,3.0411038491
H,-3.296690378,-0.0391221071,3.7088898335
H,-3.0311788498,2.237743808,2.9638970975
H,-2.8842051341,3.507814188,1.2044788888
H,-2.8842051341,3.507814188,-1.2044788888
H,-3.0311788498,2.237743808,-2.9638970975
H,-3.296690378,-0.0391221071,-3.7088898335
H,-3.5331196288,-2.0971421746,-3.0411038491
H,-3.698865653,-3.5305936098,-1.1002926026
Be,-1.9424403378,-5.7718083002,0.
H,-0.7527909564,-6.3985916753,0.
H,-3.2940084437,-5.8530669381,0.
Cl,0.6757614112,-0.4381493827,0.

Table S3. AIM parameters (in au) for the BCPs corresponding to the intermolecular interactions in the BeH₂: C_xH_y binary systems, the electron density, ρ_{BCP} , its Laplacian, $\nabla^2\rho_{\text{BCP}}$, and the total electron energy density, H_{BCP} .

System	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}	Interaction
[65] BeH ₂ : C ₂₀ H ₁₀	0.0144	0.0254	-0.0008	H... π
	0.0144	0.0256	-0.0008	
[66] BeH ₂ : C ₂₀ H ₁₀	0.0160	0.0225	-0.0018	H...C
	0.0160	0.0225	-0.0018	
[65] BeH ₂ : C ₃₀ H ₁₀	0.0112	0.0226	0.0002	H... π
	0.0107	0.0226	0.0001	
[66] BeH ₂ : C ₃₀ H ₁₀	0.0162	0.0223	-0.0018	Be...C
	0.0162	0.0223	-0.0018	
[65] BeH ₂ : C ₄₀ H ₁₀	0.0106	0.0223	0.0003	H... π
	0.0100	0.0221	0.0002	
[66] BeH ₂ : C ₄₀ H ₁₀	0.0118	0.0207	-0.0002	H...C
	0.0118	0.0207	-0.0002	
[65] BeH ₂ : C ₅₀ H ₁₀	0.0105	0.0215	0.0003	H... π
	0.0102	0.0223	0.0002	
[66] BeH ₂ : C ₅₀ H ₁₀	0.0120	0.0211	-0.0002	H...C
	0.0120	0.0211	-0.0002	
[65] BeH ₂ : C ₆₀ H ₁₀	0.0100	0.0210	0.0003	H... π
	0.0098	0.0217	0.0003	
[66] BeH ₂ : C ₆₀ H ₁₀	0.0121	0.0213	-0.0002	H...C
	0.0121	0.0213	-0.0002	
[65] BeH ₂ : C ₆₀	0.0099	0.0210	0.0004	H... π
	0.0095	0.0216	0.0004	
[66] BeH ₂ : C ₆₀	0.0107	0.0203	-0.0030	H... π
	0.0107	0.0203	-0.0030	

Table S4. AIM parameters (in au) for the BCPs corresponding to the Cl \cdots C intermolecular interactions in the C_xH_y:Cl binary systems, the electron density, ρ_{BCP} , its Laplacian, $\nabla^2\rho_{\text{BCP}}$, and the total electron energy density, H_{BCP} .

C₂₀H₁₀:Cl BCP Numbers: 5

Num.	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}
4	0.0081	0.0247	0.0009
1	0.0082	0.0249	0.0009

C₃₀H₁₀:Cl BCP Numbers: 10

Num	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}
2	0.0076	0.0221	0.0007
3	0.0077	0.0221	0.0007
5	0.0071	0.0206	0.0008

C₄₀H₁₀:Cl BCP Numbers: 15

Num	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}
5	0.0074	0.0221	0.0007
8	0.0075	0.0219	0.0008
2	0.0076	0.0220	0.0008

C₅₀H₁₀:Cl BCP Numbers: 25

Num	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}
5	0.0074	0.0221	0.0007
20	0.0078	0.0230	0.0008

C₆₀H₁₀:Cl BCP Numbers: 22

Num	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}
5	0.0072	0.0217	0.0007
7	0.0077	0.0229	0.0008
10	0.0080	0.0243	0.0009

C₆₀:Cl BCP Numbers: 60

BCPs	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}
60	0.0075	0.0224	0.0007

Table S5 AIM parameters (in au) for the BCPs corresponding to the intermolecular interactions in the ternary systems, the electron density, ρ_{BCP} , its Laplacian, $\nabla^2\rho_{\text{BCP}}$, and the total electron energy density, H_{BCP} .

[65] BeH₂: C₂₀H₁₀:Cl⁻

Num	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}	Int.
1	0.0233	0.0544	-0.0045	Be... π
1	0.0233	0.0557	-0.0044	Be... π
2	0.0088	0.0279	0.0010	Cl...C
2	0.0087	0.0270	0.0010	Cl...C
1	0.0085	0.0264	0.0010	Cl...C

[66] BeH₂: C₂₀H₁₀:Cl⁻

Num	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}	Int.
1	0.0245	0.0972	-0.0021	Be... π
1	0.0089	0.0283	0.0011	Cl...C
2	0.0089	0.0276	0.0010	Cl...C
2	0.0086	0.0269	0.0010	Cl...C

[65] BeH₂: C₃₀H₁₀:Cl⁻

Num	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}	Int.
1	0.0214	0.0372	-0.0046	Be... π
1	0.0222	0.0299	-0.0049	Be... π
5	0.0078	0.0227	0.0008	Cl...C
5	0.0073	0.0212	0.0008	Cl...C

[66] BeH₂: C₃₀H₁₀:Cl⁻

Num	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}	Int.
1	0.0245	0.0930	-0.0023	Be... π
4	0.0079	0.0228	0.0008	Cl...C
1	0.0077	0.0228	0.0008	Cl...C
5	0.0073	0.0212	0.0008	Cl...C

[65] BeH₂: C₄₀H₁₀:Cl⁻

Num	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}	Int.
1	0.0226	0.0281	-0.0049	Be... π
1	0.0209	0.0391	-0.0043	Be... π
2	0.0076	0.0230	0.0008	Cl...C
1	0.0075	0.0217	0.0007	Cl...C
1	0.0075	0.0225	0.0007	Cl...C
6	0.0076	0.0222	0.0008	Cl...C
4	0.0077	0.0224	0.0008	Cl...C
2	0.0078	0.0225	0.0008	Cl...C

[66] BeH₂: C₄₀H₁₀:Cl⁻

Num	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}	Int.
2	0.0222	0.0273	-0.0053	Be...C
2	0.0075	0.0221	0.0007	Cl...C
5	0.0076	0.0225	0.0007	Cl...C
6	0.0076	0.0233	0.0008	Cl...C
3	0.0077	0.0226	0.0008	Cl...C

[65] BeH₂: C₅₀H₁₀:Cl⁻

Num	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}	Int.
1	0.0221	0.0281	-0.0048	Be... π
1	0.0212	0.0341	-0.0046	Be... π
2	0.0076	0.0229	0.0007	Cl...C
6	0.0079	0.0235	0.0008	Cl...C
2	0.0080	0.0236	0.0008	Cl...C
3	0.0075	0.0223	0.0007	Cl...C
6	0.0078	0.0231	0.0008	Cl...C
2	0.0077	0.0234	0.0008	Cl...C

[66] BeH₂: C₅₀H₁₀:Cl⁻

Num	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}	Int.
1	0.0223	0.0282	-0.0053	Be...C
5	0.0075	0.0228	0.0007	Cl...C
6	0.0078	0.0234	0.0008	Cl...C
6	0.0079	0.0233	0.0008	Cl...C

[65] BeH₂: C₆₀H₁₀:Cl⁻

Num	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}	Int.
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[66] BeH₂: C₆₀H₁₀:Cl⁻

Num	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}	Int.
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1	0.0202	0.0293	-0.0042	Be... π	2	0.0223	0.0276	-0.0053	Be...C
1	0.0210	0.0258	-0.0043	Be... π	1	0.0073	0.0225	0.0007	Cl...C
2	0.0073	0.0219	0.0007	Cl...C	4	0.0074	0.0220	0.0007	Cl...C
2	0.0078	0.0229	0.0008	Cl...C	4	0.0078	0.0234	0.0008	Cl...C
2	0.0072	0.0216	0.0007	Cl...C	2	0.0079	0.0233	0.0008	Cl...C
2	0.0077	0.0230	0.0008	Cl...C	4	0.0080	0.0244	0.0009	Cl...C
2	0.0076	0.0227	0.0008	Cl...C	5	0.0081	0.0245	0.0009	Cl...C
1	0.0071	0.0213	0.0007	Cl...C					
2	0.0079	0.0240	0.0008	Cl...C					
8	0.0080	0.0244	0.0009	Cl...C					

[65] BeH₂: C₆₀:Cl⁻

[66] BeH₂: C₆₀:Cl⁻

Num	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}	Int	Num	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}	Int
1	0.0214	0.0265	-0.0043	Be... π	2	0.0215	0.0244	-0.0050	Be... π
1	0.0203	0.0301	-0.0042	Be... π					
29	0.0074	0.0221	0.0007	Cl...C	2	0.0075	0.0230	0.0008	Cl...C
17	0.0075	0.0226	0.0008	Cl...C	58	0.0075	0.0225	0.0007	Cl...C
8	0.0076	0.0230	0.0008	Cl...C					