

Multi-FLP Approach for CO₂ Capture: Investigating Nitrogen, Boron, Phosphorus and Aluminium Doped Nanographenes and the Influence of a Sodium Cation.

Maxime Ferrer,^{a,b} Ibon Alkorta,*^a José Elguero,^a Josep M. Oliva-Enrich^c

^a Instituto de Química Médica (CSIC), Juan de la Cierva, 3, E-28006 Madrid, Spain

^b PhD Program in Theoretical Chemistry and Computational Modeling, Doctoral School, Universidad Autónoma de Madrid, 28049 Madrid, Spain

^c Instituto de Química-Física Blas Cabrera (CSIC), Serrano, 119, E-28006 Madrid, Spain

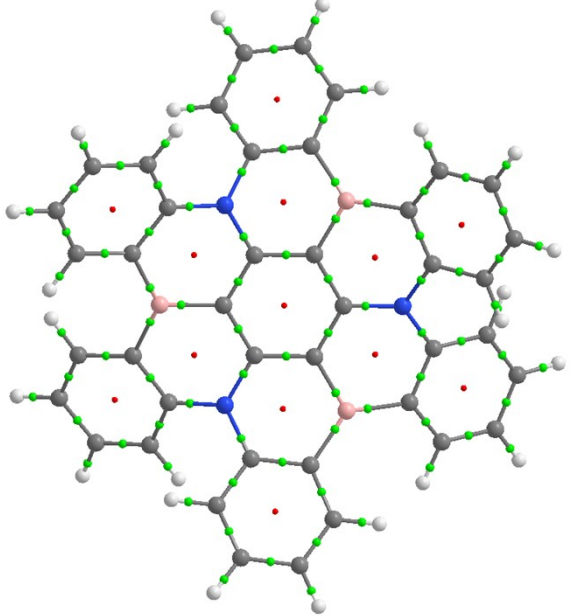
*Author to whom correspondence should be addressed: e-mail: ibon@iqm.csic.es

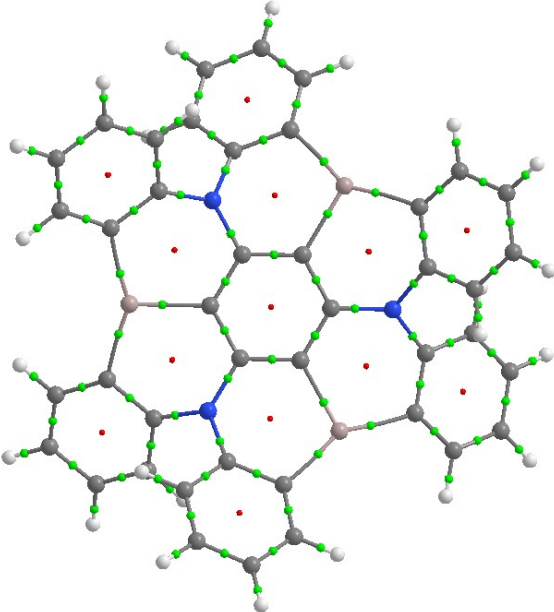
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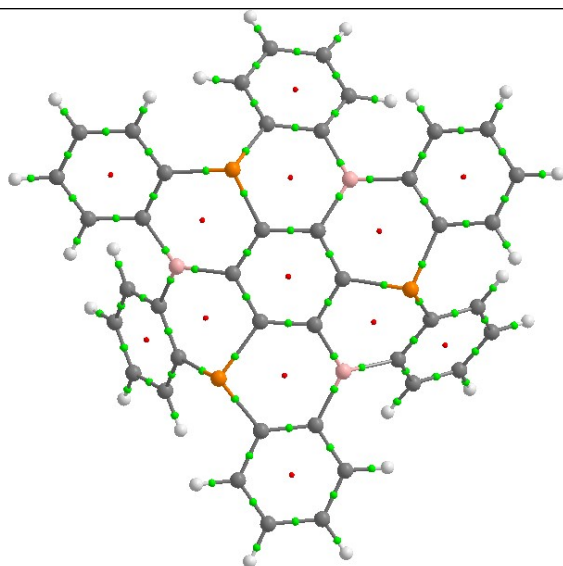
Figure S4: Comparative energy profiles of the reaction of B_3N_3 -NG and B_3P_3 -NG in the absence/presence of Na^+ with three molecules of CO_2 .

Table S1: Molecular graphs, energies (in Hartree) and Cartesian coordinates (in Å) of the monomers in vacuum. Level of theory: M06-2X/6-311++G**/M06-2X/6-31+G*

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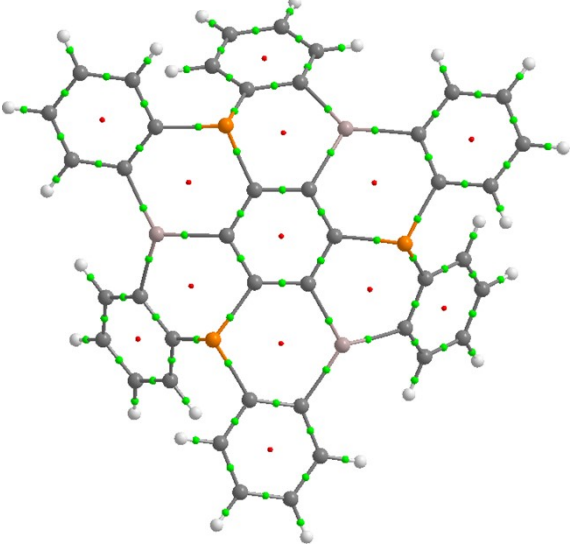
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B₃P₃-NG

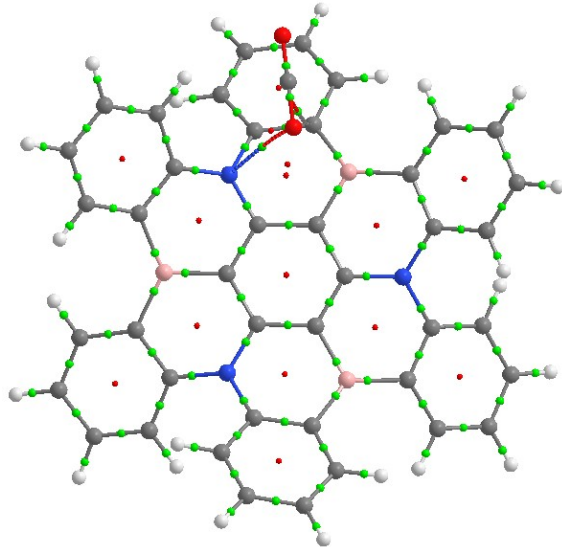
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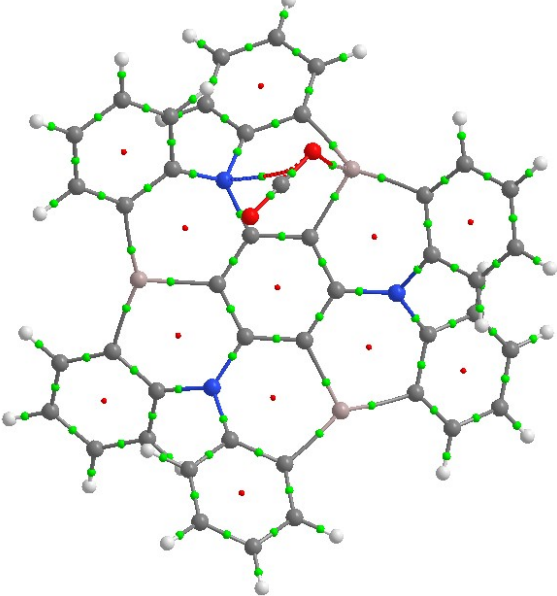
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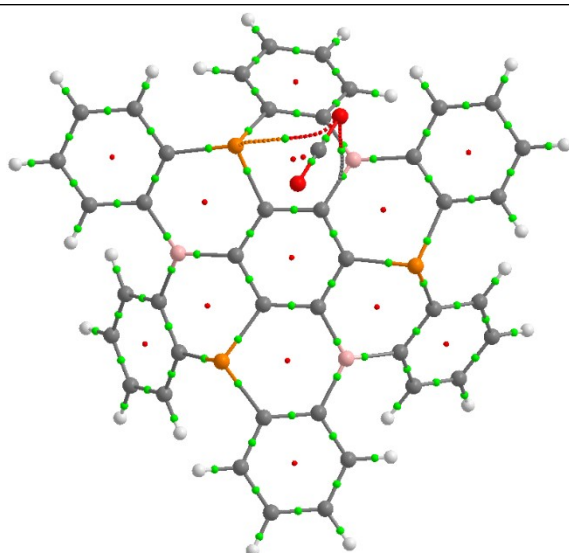
	<p> C,6.7789547865,0.1784356762,-1.1198355391 H,7.7122867412,0.6757229873,-1.3687597805 P,2.920100244,1.4124791907,-1.1008184559 C,1.1393450339,-0.856997066,-0.8745527212 C,1.9732767025,-3.5236646727,0.6408704193 C,4.1546446419,2.3997545058,1.2929422891 H,4.911855696,1.6331405164,1.1581335884 C,3.0534121562,2.4724824396,0.4347690449 C,1.2928834623,0.5314417726,-0.8694719377 C,2.6609952218,-4.1112877438,1.7122262309 H,3.6988590775,-3.8385809645,1.9000717113 C,2.0649447686,3.4707400877,0.6408704193 C,0.6145265259,-3.8805737171,0.4347690449 C,0.0009260448,-4.7979050584,1.2929422891 H,-1.041586672,-5.0703620725,1.1581335884 C,2.0515162734,-5.0420828136,2.5548577153 C,4.2950718964,3.3082643674,2.3447137704 H,5.1562274754,3.2319875628,3.0032547855 C,3.3408136667,4.2977066141,2.5548577153 C,2.2299820163,4.3601333316,1.7122262309 H,1.4748790898,5.1225964066,1.9000717113 C,0.7175050373,-5.3737735589,2.3447137704 H,0.2208695973,-6.0814177646,3.0032547855 C,-4.8909772383,-0.2488455914,1.7122262309 H,-5.1737381676,-1.2840154457,1.9000717113 H,-3.8702690243,3.4372215526,1.1581335884 H,-5.3770970729,2.8494301983,3.0032547855 H,-5.3265369381,-5.8342862085,-0.6060532049 H,-6.0633093963,0.4877191085,3.3697013277 H,-2.3893715995,7.530059405,-0.6060532049 H,3.4540318369,5.0071204121,3.3697013277 H,7.7159085374,-1.6957732001,-0.6060532049 H,2.6092775591,-5.4948395241,3.3697013277 Al,2.6186860911,-1.9563655524,-0.3118850735 Al,-3.0036053121,-1.2896659051,-0.3118850735 Al,0.3849192207,3.2460314539,-0.3118850735 </p>
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Table S2: Molecular graphs, energies (in Hartree) and Cartesian coordinates (in Å) of the complexes in vacuum. Level of theory: M06-2X/6-311++G*//M06-2X/6-31+G*

	<p>B₃N₃-NG:CO₂ E=-2042,35849833H; FreqIm=0</p> <p>C,3.7691300511,-4.9092887732,1.4419191275 C,1.5036316179,-3.4973547201,0.5668282909 C,2.783746287,-2.9189187479,0.419028982 C,1.3674823637,-4.7487340318,1.1934985884 C,2.4883579915,-5.4451145068,1.6156653091 C,1.5457824196,-0.7011411922,0.0789208706 C,4.0291922955,-0.5946771178,-0.5429991682 C,1.5052609471,0.711169465,0.0710650721 C,-0.663324242,-4.7504754159,-0.8984024315 H,0.3302380161,-5.1456214449,-1.0785555237 C,-0.8236223322,-3.5125507692,-0.2509206084 C,0.3200166403,-1.3972698452,0.1740545065 C,5.1748107062,-1.1422056885,-1.1538783071 H,5.2989116069,-2.2219563592,-1.1469464055 C,-2.114562194,-2.9594670862,-0.1014105177 C,3.8525210717,0.8056364647,-0.5996637786 C,4.7768335827,1.6003898446,-1.3010576377 H,4.6058199851,2.6654988714,-1.4104090139 C,6.1109062214,-0.3551869852,-1.8032961527 B,2.8526829625,-1.4416331071,-0.018293938 C,-1.7699485245,-5.4561591616,-1.3424167222 H,-1.6223268651,-6.4039569554,-1.8521827237 C,-3.0607711977,-4.9442989883,-1.1701277582 C,-3.2137879192,-3.7050909034,-0.5711598528 H,-4.2075160926,-3.2704956071,-0.4917465941 C,5.8932132346,1.0245407785,-1.8853425617 H,6.5874640593,1.6553819327,-2.4331097917 B,-2.2100657936,-1.4907305522,0.3542646128 C,-0.9179865556,-0.7251754165,0.272136446 C,-2.4802779813,5.2831121766,-1.2419127139 C,-2.2304631275,2.7001642505,-0.1574108801 C,-1.1005791326,3.5464948819,-0.2120133043 C,-1.2624492614,4.8346864463,-0.7583175558 H,-0.3886676213,5.4764936131,-0.8361158907 C,-3.4586474907,3.1407882468,-0.6838600591 H,-4.322062322,2.4839746724,-0.6931215551 C,-3.5779441567,4.4168960099,-1.2113373504 H,-4.5333600961,4.72983685,-1.6227224848 C,0.2892362455,1.4266349514,0.1566572298 C,1.6275274314,3.5920803765,0.445845142 C,-4.2111488725,1.5158026784,1.6045776733 H,-4.062334095,2.5847038752,1.7103373444 C,-3.2614203597,0.736386088,0.9206911828 C,-0.9096504316,0.686729849,0.2593783671 C,1.7612496332,4.9033907886,0.9434574207 H,0.8762303605,5.5327741686,0.9886973305 C,-3.4091006837,-0.6681902985,0.8698691984 C,2.7734179286,2.7664802349,0.4357143698 C,3.9852204104,3.2429198012,0.966440775 H,4.8469620814,2.5875751186,1.0277028369 C,2.9661930921,5.3900734406,1.4220719783</p>
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	<p>B,0.2715455021,2.9308694215,0.1278781788 C,-5.327080571,0.9210436238,2.1699106176 H,-6.0445619115,1.5405111336,2.7003334184 C,-5.5175437873,-0.4628299575,2.0892665331 C,-4.5548733389,-1.2354341458,1.4624352167 H,-4.6589398062,-2.3173410749,1.4567734824 C,4.0775863664,4.5402382661,1.4438555587 H,5.0197819734,4.8840658007,1.8610387793 C,3.8978323167,-3.656421703,0.8660630554 H,4.8827722332,-3.2030831319,0.7905323163 H,0.3813105346,-5.162467058,1.373077981 H,2.3599599168,-6.4042834762,2.1091439264 O,-2.9490975277,-0.0583305108,-2.3065280448 C,-4.0805455474,0.0652678122,-2.06797478 O,-5.2156676833,0.193731382,-1.8440230591 H,6.9814303597,-0.8031213116,-2.272558212 H,-2.5763863658,6.2779105387,-1.6657805455 H,-6.3901667707,-0.924219855,2.5410628217 H,-3.9234479961,-5.4960565623,-1.5306752928 H,4.6436102063,-5.4535608915,1.7850068075 H,3.0408550813,6.4023034027,1.8074048571 N,-2.1225232647,1.372008371,0.3479031602 N,2.701139576,1.4211902744,-0.0286987173 N,0.3323286095,-2.7920215493,0.1664015677</p>
	<p>Al₃N₃-NG:CO₂ E=-2694,93518542H; FreqIm=0 C,3.0209041663,-5.3902500543,2.0512020539 C,1.2266406381,-3.6146064918,0.7857393219 C,2.6221110419,-3.3626265906,0.7309711378 C,0.7620976846,-4.7321889169,1.5055958786 C,1.6427855442,-5.6064530247,2.1235803923 C,1.4077202165,-0.683092133,0.1248574836 C,4.2979420014,-0.2968856257,-0.5689266611 C,1.3610214569,0.7226191608,0.123906841 C,-0.2713741249,-4.6960417601,-1.3238956685 H,0.8034493122,-4.8404404688,-1.3842063499 C,-0.776306176,-3.6215201013,-0.5666576647 C,0.1932418759,-1.3959517995,0.1446292794 C,5.5021905708,-0.5549201113,-1.2516947069 H,5.9246197249,-1.5572820179,-1.2097214575 C,-2.1784272376,-3.412185533,-0.5159419064 C,3.7602922257,1.0145434081,-0.6364936749 C,4.4237803324,1.9846576684,-1.4125490437 H,3.9996354952,2.9814730131,-1.4892639071 C,6.1720150954,0.418307026,-1.9804453774 C,-1.1179814622,-5.5768421452,-1.9802101688 H,-0.6933324932,-6.3946006859,-2.5559078611 C,-2.5016081054,-5.40553651,-1.9116390662 C,-3.0042072434,-4.3230637931,-1.2009256463 H,-4.0824502568,-4.1740958877,-1.1760565387 C,5.6096837236,1.6935851875,-2.0692075941 H,6.0924051004,2.4656387777,-2.6619441062 C,-1.0447600427,-0.7373982093,0.1727276043 C,-3.4634944425,4.9496301451,-1.6727420942 C,-2.6135067168,2.5787846704,-0.3929937492 C,-1.7278788141,3.684029841,-0.4860206042</p>

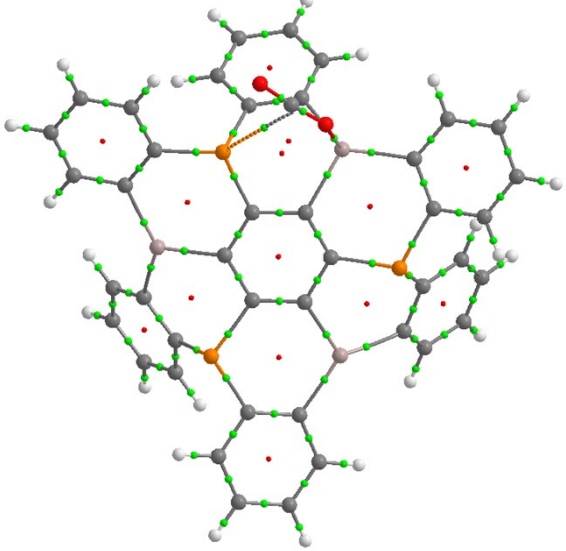
	<p> C,-2.188806182,4.8467743471,-1.1335876033 H,-1.5199541624,5.7017993322,-1.214548133 C,-3.9008852766,2.6841631218,-0.9598833147 H,-4.5805334597,1.8383439791,-0.8893562324 C,-4.3183784278,3.8481726651,-1.5861928733 H,-5.3153825732,3.8927709087,-2.0158378264 C,0.1377430703,1.41807161,0.1753449894 C,1.8395149208,3.8415597638,0.597765125 C,-3.9751462724,1.7964707297,1.9664825239 H,-3.5875000055,2.811525098,1.9763240535 C,-3.393450141,0.8473323525,1.111164696 C,-1.0451670603,0.6648119508,0.2099911019 C,2.2022345769,5.0648206538,1.1930008503 H,1.5098525896,5.9027496693,1.1353372682 C,-3.8793256762,-0.4822048746,1.1011595577 C,2.7542177921,2.7602573195,0.6869293207 C,3.95653933,2.9385414603,1.3965855587 H,4.6449994457,2.1032076197,1.4859542807 C,3.4088351721,5.2446198029,1.8560552511 C,-5.0422616171,1.4559095433,2.7873053426 H,-5.4732237932,2.2076157848,3.4426801728 C,-5.5469936384,0.1553752754,2.7783719317 C,-4.9531512446,-0.7926395508,1.9518563349 H,-5.3381194009,-1.8105005281,1.9661511351 C,4.2806975555,4.1595900069,1.9682345333 H,5.2156949738,4.2614822384,2.5120533844 C,3.484775035,-4.2703473431,1.3748985809 H,4.5575002146,-4.0881212913,1.3432233039 H,-0.3071651817,-4.9120698523,1.5683536515 H,1.2497281642,-6.4565594736,2.6742943043 H,-3.7873493928,5.8640293143,-2.1605506852 H,-6.3826562221,-0.1156036436,3.4170162608 H,3.6608787069,6.2043305252,2.2972307133 H,3.7141397866,-6.0751542793,2.53027942 H,7.1037412576,0.1878436625,-2.4883534346 H,-3.1704920726,-6.094009831,-2.4196078878 O,-1.746976897,0.7515771175,-2.9558469021 C,-2.4863484013,0.0348111358,-2.4368258248 O,-3.2574938161,-0.7045332919,-1.9468325683 N,2.5850336341,1.4700534979,0.0632086975 N,0.2152116315,-2.8317870875,0.1251460465 N,-2.3271584284,1.3289001848,0.252666797 Al,0.0755215398,3.2890008048,0.0630557666 Al,-2.6931813801,-1.6675129219,0.1353527642 Al,3.048007236,-1.5962805447,0.0999714219 </p>
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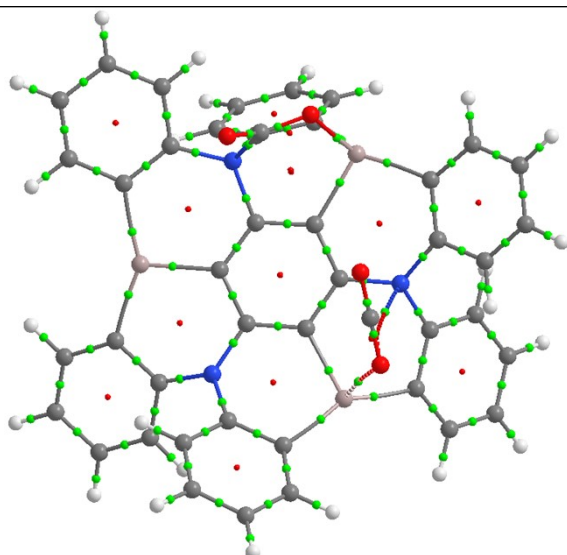
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 C,0,-4.240492,-0.555346,0.843341
 C,0,-1.488862,0.327376,0.701673
 C,0,-0.453646,5.339316,0.261433
 H,0,-1.525127,5.503529,0.1845
 C,0,-3.727244,-1.840245,0.546445
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 C,0,2.272484,4.949714,0.571364
 H,0,3.336001,4.801479,0.74981
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 C,0,-5.983937,-2.746535,0.848749
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 H,0,-4.255424,-3.925556,0.404699
 C,0,1.763359,6.242435,0.515406
 H,0,2.432543,7.092805,0.61113
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 C,0,-1.135786,-1.024327,0.645035
 C,0,5.141087,-3.70054,0.084374
 C,0,2.387918,-3.288499,0.377695
 C,0,3.215776,-2.186054,0.063783
 C,0,4.599239,-2.428445,-0.051867
 H,0,5.265012,-1.58781,-0.228553
 C,0,2.940506,-4.568465,0.535642
 H,0,2.302404,-5.401217,0.826085
 C,0,4.302968,-4.781519,0.361074
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	<p>B,0,2.658892,-0.731236,-0.067884 C,0,-0.786624,-5.361136,-2.298403 H,0,-0.418976,-6.143698,-2.956504 C,0,-2.080551,-4.869059,-2.44812 C,0,-2.533944,-3.860141,-1.601543 H,0,-3.536772,-3.466075,-1.743934 C,0,4.533257,2.288786,-2.655674 H,0,4.964053,3.035393,-3.317187 C,0,-2.521357,3.852443,-1.622721 H,0,-1.701947,4.512217,-1.895624 H,0,-5.41805,1.432309,-0.791282 H,0,-5.677668,3.080905,-2.605202 O,0,2.018085,0.278314,3.836578 C,0,2.935856,0.0561,3.160306 O,0,3.863844,-0.181351,2.496211 H,0,-0.022438,7.443588,0.374399 H,0,-3.806286,4.619442,-3.171711 H,0,-6.651117,-3.603335,0.868432 H,0,-2.730903,-5.263774,-3.223146 H,0,6.213009,-3.849349,-0.007808 H,0,5.31796,0.612519,-3.759464</p>
	<p>Al₃P₃-NG:CO₂ E=-3554,73212323H; FreqIm=0 C,-3.649910148,4.2823721151,2.3998146868 C,-1.8312448994,3.5381747771,0.386687511 C,-3.0811043362,2.8720370166,0.4867399224 C,-1.511102653,4.5486168283,1.2983698018 C,-2.4166831236,4.9168601543,2.2961562757 P,-2.6846809084,-2.1255087535,-1.2730456284 P,-0.7455290414,3.1436671589,-1.0858367848 C,-1.5160389166,0.5033177526,-0.9386798178 C,-4.7042222832,-0.0266235632,-0.8391810686 C,-1.3393702961,-0.882697735,-0.922546333 C,0.4807482624,5.5639467287,-1.0671310856 H,-0.5015839219,5.8603740677,-1.4321059138 C,0.7373917022,4.2106948526,-0.7835829913 C,-0.3589824385,1.3334489916,-0.8490949161 C,-6.0628583552,0.3384362201,-0.860820483 H,-6.3492318028,1.3493869809,-0.5737662652 C,2.0250939087,3.8182820649,-0.3545164632 C,-4.3620613426,-1.3427687001,-1.2292712833 C,-5.370889474,-2.2228711731,-1.6554044074 H,-5.1053335589,-3.225913086,-1.985584412 C,-7.061134674,-0.552064535,-1.2454745548 C,1.4565527521,6.5360494239,-0.8760130449 H,1.2306724904,7.5774633045,-1.0878954946 C,2.7243107305,6.1668541334,-0.4263752478 C,2.9959627124,4.822999345,-0.187098314 H,3.9992716761,4.5465254916,0.1371172342 C,-6.7083244319,-1.8391435692,-1.6500611168 H,-7.4723368508,-2.5416027445,-1.9713815534 C,0.9307599037,0.8030659592,-0.7675392758 C,3.6299427522,-5.7332102047,-0.2419992329 C,2.9804483784,-3.016596335,-0.5411557798 C,1.9572238649,-3.9447212554,-0.2366823518 C,2.3156926812,-5.2979110186,-0.0965517968</p>

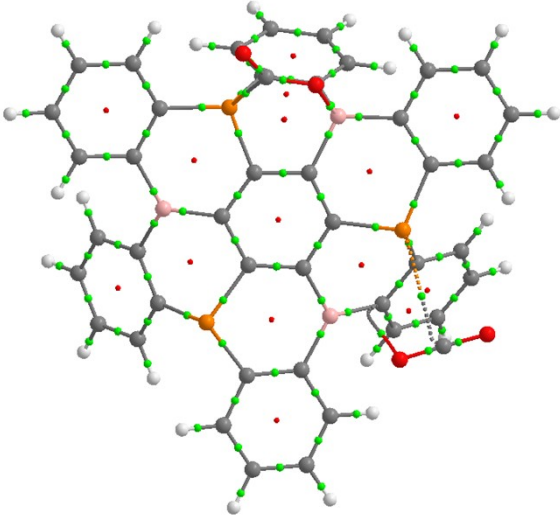
	<p> H,1.5453686204,-6.0343025878,0.1283477226 C,4.2986386248,-3.4663980105,-0.7216948808 H,5.0803690492,-2.7543823015,-0.9826240936 C,4.62489851,-4.8094395807,-0.5604799727 H,5.6528854797,-5.1347336106,-0.6933086179 P,2.8237496406,-1.187840666,-0.7406619862 C,-0.0466526357,-1.4722508307,-0.8127226029 C,-1.5246063662,-3.9184821023,0.58470176 C,4.0629596534,-1.3562085097,1.8393013881 H,4.0427600325,-2.4364604877,1.7244092555 C,3.4958257869,-0.5246618615,0.868905233 C,1.0543536814,-0.6162433123,-0.7265592326 C,-1.5706346074,-4.8203747788,1.6574379942 H,-0.6762200515,-5.3797969808,1.929300321 C,3.5136211929,0.8851848853,1.0294358241 C,-2.6993062837,-3.1857687874,0.2684270829 C,-3.8599542129,-3.3784303295,1.0236872849 H,-4.7622800413,-2.8152415782,0.8049039062 C,-2.7367174629,-5.0246079052,2.3965942765 C,4.6558021237,-0.8046345485,2.9768765671 H,5.0890462847,-1.4616982994,3.7262740068 C,4.6842030637,0.5748131671,3.1548237687 C,4.1047520824,1.4019723708,2.190650871 H,4.1142715893,2.4791252951,2.3538514916 C,-3.8758287114,-4.2926207326,2.0796336984 H,-4.7869482671,-4.4236187306,2.6574018351 C,-3.9631591018,3.2570074899,1.5063243134 H,-4.9198877205,2.7466755363,1.6118133991 H,-0.5521795202,5.0556073849,1.2476289329 H,-2.1464640211,5.7020474255,2.9973479903 H,3.8766066418,-6.7843864994,-0.1222475994 H,5.1466135282,1.0037462647,4.0395454994 H,-2.7515635403,-5.7391226717,3.2147115387 H,-4.3555709276,4.5738829151,3.1726147355 H,-8.1026810819,-0.243219202,-1.2459376275 H,3.4949358239,6.9187555754,-0.2802282849 O,5.3586764019,0.2523046539,-2.7300272977 C,4.5508985167,0.9602117878,-2.3145821309 O,3.7765718068,1.7629080092,-1.9387879471 Al,2.4242516575,1.9231980571,-0.229861814 Al,-3.2561935189,1.2140983883,-0.5116258707 Al,0.1313329215,-3.2973279946,-0.2223765529 </p>
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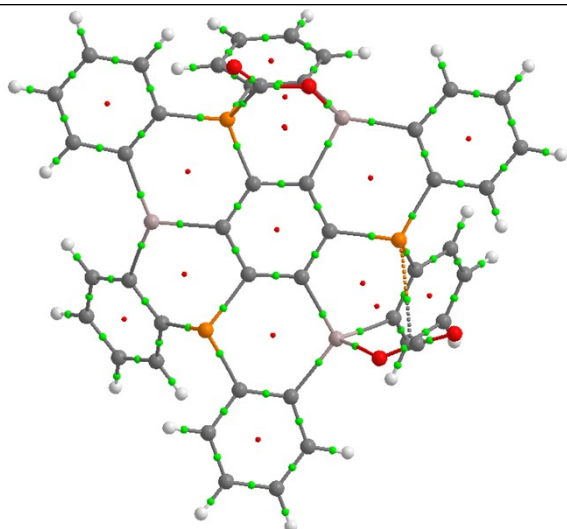
1CO₂-Al₃N₃:CO₂

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 C,-2.0118034374,3.806673914,0.6059192384
 C,-0.0472432463,4.901837158,1.5392238044
 C,-0.841652037,5.9012912958,2.0771683112
 C,-1.1735176596,0.9873803714,0.0219335699
 C,-4.1502606826,0.9946713798,-0.5126511608
 C,-1.2874690829,-0.396186669,-0.0205978954
 C,1.2635075774,4.680172933,-1.1503036788
 H,0.2375942102,4.9936815544,-1.3206513673
 C,1.50954121,3.5418025775,-0.3597042093
 C,0.1313335861,1.50133669,0.2005613199
 C,-5.4495085283,1.4396991799,-0.8362068155
 H,-5.6691630123,2.5037016635,-0.7749716659
 C,2.8462577551,3.1074537948,-0.1688918481
 C,-3.90666285,-0.38398551,-0.6047705296
 C,-4.9206004517,-1.2618236221,-1.0081876594
 H,-4.7197521891,-2.329400441,-1.0640152056
 C,-6.4596309363,0.5758292211,-1.23123661
 C,2.3034115507,5.4131139826,-1.7026656791
 H,2.0772009164,6.2865232252,-2.3079590704
 C,3.6267200648,5.0221997073,-1.4933470031
 C,3.8731188195,3.8734415115,-0.7520646321
 H,4.9052051451,3.5527282612,-0.620786619
 C,-6.1843661261,-0.7900985002,-1.3208844086
 H,-6.9534919037,-1.4892677306,-1.6341999318
 C,1.235127038,0.650936939,0.3411452133
 C,2.7875125431,-5.4007945791,-1.3532172214
 C,2.2493217391,-2.9130720735,-0.1416523005
 C,1.1916720907,-3.8441910229,-0.3109632172
 C,1.5074601756,-5.0720510751,-0.9227977203
 H,0.7128482724,-5.8013649758,-1.071337248
 C,3.538731654,-3.237105224,-0.6061615924
 H,4.3430725868,-2.5161014193,-0.478204346
 C,3.8077593025,-4.4628298457,-1.1976009249
 H,4.8147318299,-4.6798155316,-1.5433230125
 C,-0.2397824024,-1.2882747192,0.1102762924
 C,-2.1698297111,-3.1698410858,1.1865501258
 C,3.5470372996,-2.369146252,2.3179942462
 H,3.0090248981,-3.3111124206,2.2611519778
 C,3.1964008172,-1.3252181287,1.4454834571
 C,1.0267234634,-0.7395512825,0.3189293973
 C,-2.5069344788,-3.9288926593,2.3140615469
 H,-1.9429393508,-4.8347531535,2.5252233517
 C,3.8804999867,-0.0865179721,1.5256036102
 C,-2.9318747246,-2.0097356307,0.9551598749
 C,-3.9297186492,-1.5961018866,1.84009606
 H,-4.4897566704,-0.6824470521,1.6777724531
 C,-3.5234554286,-3.5545927422,3.1907360609
 C,4.5723983147,-2.2136091602,3.2403801165
 H,4.8204875364,-3.0363112662,3.9052261916
 C,5.2689390482,-1.007107304,3.3220053298
 C,4.9057064464,0.0366284907,2.4788028342
 H,5.4387940468,0.9820039115,2.560743187

	<p>C,-4.220541264,-2.3736604055,2.9591576444 H,-4.9967409591,-2.0458107074,3.6440686104 C,-2.7865117479,4.8387079892,1.1721835352 H,-3.8676828049,4.8127934695,1.0473055456 H,1.0265549117,4.9253602899,1.6987540741 H,-0.3779113848,6.6911478452,2.6614986218 O,-2.5622255453,-1.273149526,-2.6862657857 C,-2.2521468341,-1.9263712681,-1.7475261241 O,-1.7002944806,-3.0328646459,-1.5540175747 O,3.5921967023,0.2876618356,-1.5434553062 C,2.7904624769,-0.3370797926,-2.135783773 O,2.0238026084,-0.9385672729,-2.7506013015 H,-7.4480972528,0.955341573,-1.4719625338 H,4.4464202261,5.5930975607,-1.9194590697 H,-2.8504184506,6.6717384456,2.3028066209 H,6.0733493925,-0.8820238749,4.0408884998 H,-3.7554607669,-4.167230232,4.057353671 H,2.9859986464,-6.3635551016,-1.8149204234 Al,3.0154181669,1.2939549778,0.4845001863 Al,-2.6542792502,2.1257774335,-0.0548249829 Al,-0.6136278853,-3.1724827739,-0.013667473 N,2.1515664709,-1.6136258997,0.486949728 N,0.3368567003,2.9228350078,0.2166974797 N,-2.6385233834,-1.1083322895,-0.249796792</p>
	<p>1CO₂-B₃P₃:CO₂ E=-3090,65678173H; FreqIm=0 C,0,-3.133258,4.883517,2.004378 C,0,-1.163562,3.933814,0.248268 C,0,-2.392716,3.228989,0.359505 C,0,-0.952884,5.101637,0.983112 C,0,-1.928659,5.568801,1.862361 P,0,-2.916998,-1.278648,-0.406191 P,0,0.044736,3.344702,-1.00835 C,0,-1.329912,1.007858,-0.648695 C,0,-4.039822,1.225035,-0.573891 C,0,-1.383755,-0.38626,-0.604111 C,0,2.044139,5.209015,-0.695277 H,0,1.273362,5.91266,-1.003892 C,0,1.724187,3.853962,-0.522246 C,0,-0.026759,1.566539,-0.67949 C,0,-5.135385,2.060858,-0.842964 H,0,-4.985411,3.137091,-0.856224 C,0,2.73494,2.915328,-0.201398 C,0,-4.298801,-0.168556,-0.612132 C,0,-5.564432,-0.695071,-0.878286 H,0,-5.712378,-1.771017,-0.922351 C,0,-6.403309,1.549139,-1.119133 B,0,-2.601503,1.844895,-0.335723 C,0,3.34638,5.662007,-0.519031 H,0,3.574887,6.716566,-0.644687 C,0,4.360652,4.75007,-0.226492 C,0,4.051472,3.403274,-0.082152 H,0,4.854861,2.696274,0.106649 C,0,-6.624525,0.173864,-1.126646 H,0,-7.610894,-0.223661,-1.343994 B,0,2.450944,1.383291,-0.055373</p>

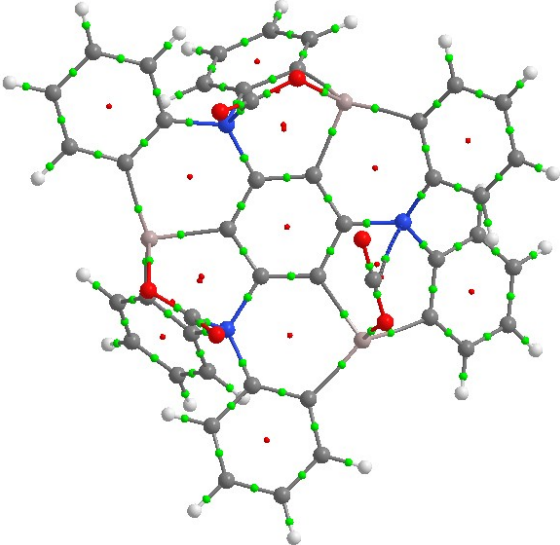
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C,0,1.998109,-3.369516,-0.485789
C,0,0.661094,-3.806642,-0.39627
C,0,0.442895,-5.192985,-0.324481
H,0,-0.583605,-5.551862,-0.266895
C,0,3.050016,-4.300696,-0.537004
H,0,4.072349,-3.954633,-0.685004
C,0,2.801458,-5.664018,-0.436071
H,0,3.626021,-6.370647,-0.465665
P,0,2.480599,-1.635345,-0.813634
C,0,-0.292277,-1.262115,-0.608581
C,0,-1.480669,-2.929176,1.041347
C,0,4.097983,-1.782606,1.520218
H,0,4.103407,-2.859728,1.380308
C,0,3.363004,-0.965559,0.659274
C,0,0.963929,-0.655603,-0.630563
C,0,-1.139074,-3.657302,2.184552
H,0,-0.215828,-4.231952,2.191006
C,0,3.347399,0.443022,0.836438
C,0,-2.684714,-2.200721,1.117961
C,0,-3.529727,-2.188481,2.224096
H,0,-4.448079,-1.605845,2.222782
C,0,-1.963028,-3.661549,3.3136
B,0,-0.60854,-2.835789,-0.358217
C,0,4.791199,-1.229301,2.595464
H,0,5.339486,-1.879139,3.272057
C,0,4.760191,0.14571,2.814268
C,0,4.047065,0.962658,1.940845
H,0,4.008673,2.031131,2.136044
C,0,-3.155387,-2.937338,3.338529
H,0,-3.78685,-2.950194,4.22164
C,0,-3.353815,3.730924,1.257034
H,0,-4.284882,3.186764,1.394237
H,0,-0.009898,5.635068,0.906044
H,0,-1.736777,6.462872,2.449221
O,0,-3.618451,-2.914285,-2.468856
C,0,-2.74211,-2.683577,-1.674154
O,0,-1.616204,-3.287146,-1.489618
O,0,4.421058,0.817573,-2.150684
C,0,5.085128,-0.125987,-1.989083
O,0,5.773793,-1.049023,-1.833358
H,0,-7.222065,2.229656,-1.334111
H,0,5.388496,5.087275,-0.129789
H,0,-3.88938,5.239675,2.697473
H,0,5.282965,0.578732,3.662043
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H,0,1.273804,-7.178533,-0.274173



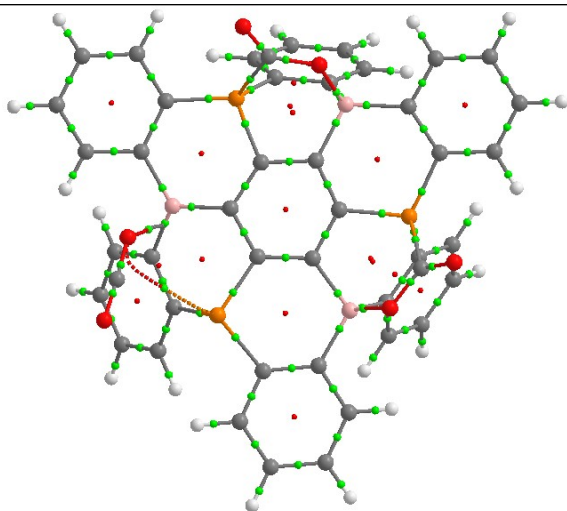
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 C,-0.3346668511,5.0583577435,1.2148982267
 C,-1.1422881348,5.7039321258,2.154076774
 P,-2.9418588394,-1.2757687406,-0.5380222615
 P,0.118815786,3.370241327,-1.0631136075
 C,-1.2433509653,0.9949782264,-0.7243676642
 C,-4.4616622432,1.1255719649,-0.5711927062
 C,-1.3427630627,-0.3948167093,-0.6266990135
 C,1.8786673302,5.4344038843,-1.0951038142
 H,0.9886433311,5.9488174328,-1.4549948091
 C,1.8128573402,4.0641038046,-0.7849188639
 C,0.0689214777,1.5376749538,-0.7291622323
 C,-5.714063391,1.7557063348,-0.6526889809
 H,-5.7775972876,2.8369722324,-0.5431833368
 C,2.9805367666,3.3830307968,-0.3706688197
 C,-4.4451391664,-0.2819482669,-0.7267969601
 C,-5.6195594991,-1.0096186487,-0.9579525069
 H,-5.5828860047,-2.0873358268,-1.0896279866
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 C,3.0593863271,6.151809137,-0.9386641579
 H,3.0816938691,7.2129601212,-1.170704821
 C,4.2118371141,5.5010786985,-0.4988109585
 C,4.1628818682,4.1349580523,-0.2377105617
 H,5.0793235124,3.634793342,0.0753927452
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 C,1.2012072026,0.7137480193,-0.6747323587
 C,2.3260281732,-6.3011016445,-0.3926319295
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 C,1.1284475555,-5.5957220837,-0.3148469809
 H,0.2035321498,-6.1615829462,-0.2082789904
 C,3.4979014034,-4.213918188,-0.6391722091
 H,4.4338168768,-3.677014261,-0.7910982983
 C,3.520330402,-5.6015999263,-0.5588641187
 H,4.4644632313,-6.1330515063,-0.6397712122
 P,2.5783154231,-1.677291924,-0.6847429361
 C,-0.252983902,-1.2866769787,-0.5703176753
 C,-1.9450884769,-3.1663793822,1.1906444558
 C,3.818897344,-2.1072622609,1.8654415068
 H,3.5379687812,-3.1524825105,1.7694077245
 C,3.4393546463,-1.1786994537,0.8925556274
 C,1.0095841328,-0.6931181623,-0.6002924288
 C,-1.9666431548,-3.8812959536,2.3950111564
 H,-1.1911939371,-4.6198783869,2.590022552
 C,3.7924718707,0.1901446182,1.02635754
 C,-2.981684613,-2.2201573206,1.020221065
 C,-3.9811903612,-1.9950930502,1.9705114263
 H,-4.7618842963,-1.2571160354,1.8009691627
 C,-2.9555675107,-3.6767508014,3.3602888781
 C,4.5548384588,-1.6965915372,2.9787482066
 H,4.8401499546,-2.4273606257,3.7308673448

	<p>C,4.9125822101,-0.3605711445,3.1301106495 C,4.518874717,0.5678050828,2.1642454231 H,4.7867550281,1.614198191,2.3076335653 C,-3.961863645,-2.7354326321,3.1512077767 H,-4.7290409317,-2.574569968,3.9027897045 C,-3.0329680511,4.4247081787,1.4111781568 H,-4.0875159052,4.1711534255,1.5133647129 H,0.7205878557,5.3096733517,1.1718179583 H,-0.7006160139,6.4433908105,2.81671611 O,-3.7168417465,-2.6904534642,-2.7197153978 C,-2.8534190914,-2.6578246662,-1.8785374762 O,-1.8492334839,-3.4407994705,-1.7031985794 O,4.1179857509,0.953393654,-1.9665035644 C,4.6404985222,-0.0207321854,-2.376519279 O,5.2289990035,-0.8947040873,-2.8391686735 H,-7.840072269,1.5601585785,-0.9395283018 H,5.1409432551,6.0514469142,-0.3791145127 H,-3.1246118978,5.9102631489,2.9756062274 H,5.4864262633,-0.0415323022,3.9958571305 H,-2.941273208,-4.2536075292,4.2812944209 H,2.3288412288,-7.386360957,-0.3389482647 Al,2.9504215534,1.4436518512,-0.2269193874 Al,-2.7809433446,2.1094531887,-0.3939852252 Al,-0.6213082021,-3.208344139,-0.3154884963</p>
	<p>2CO₂-Al₃N₃:CO₂ E-3072,11172002H; FreqIm=0 C,-5.37949,1.695833,2.753099 C,-3.138505,1.840735,1.058773 C,-3.967249,0.691428,1.02189 C,-3.43426,2.882313,1.95325 C,-4.543223,2.812657,2.785214 C,-1.342807,-0.326322,0.028154 C,-3.197379,-2.657902,-0.349437 C,-0.324087,-1.244256,-0.099628 C,-3.05353,3.871445,-0.913117 H,-3.949928,3.255344,-0.898318 C,-1.862846,3.358137,-0.363745 C,-0.962744,1.035166,0.101532 C,-4.359572,-3.433206,-0.549968 H,-5.330923,-2.951531,-0.454773 C,-0.683826,4.149155,-0.38843 C,-1.970192,-3.324226,-0.478865 C,-1.919024,-4.68406,-0.810756 H,-0.956117,-5.181393,-0.906449 C,-4.321185,-4.783045,-0.866582 C,-3.113195,5.150013,-1.447093 H,-4.049598,5.513881,-1.860952 C,-1.972926,5.953098,-1.459325 C,-0.788089,5.437406,-0.94796 H,0.102254,6.062769,-0.987132 C,-3.081818,-5.410289,-1.004528 H,-3.019104,-6.462786,-1.26308 C,0.369225,1.420375,0.01153 C,6.335703,-1.265428,-1.136264 C,3.91838,0.020937,-0.569666 C,3.932956,-1.38365,-0.608347</p>

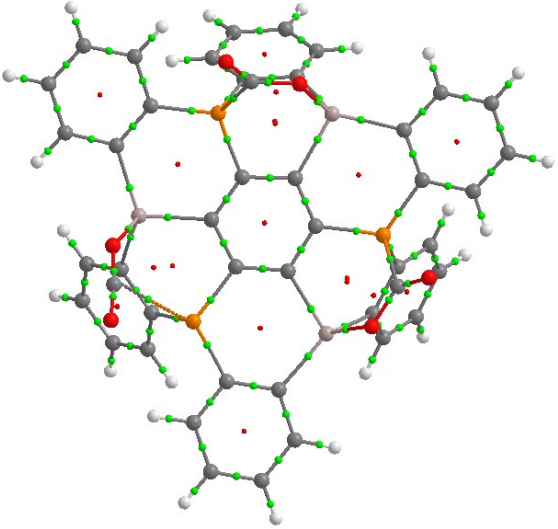
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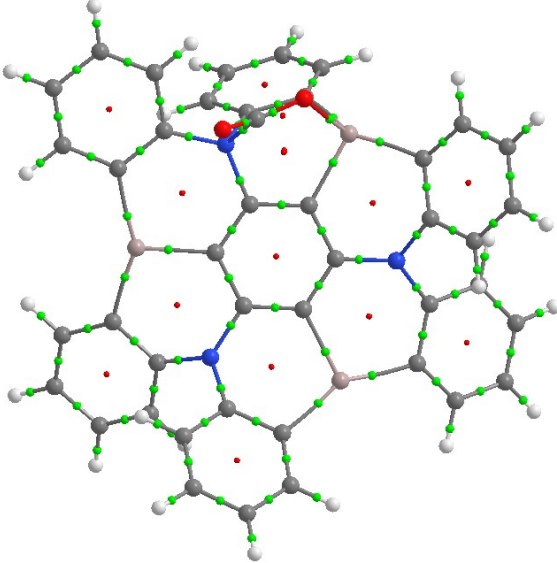
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	<p>B,0,2.611304,-1.598847,-0.492001 C,0,2.898273,3.369316,3.189981 H,0,3.569431,3.445542,4.040091 C,0,1.643882,3.977771,3.225295 C,0,0.76882,3.888385,2.138576 H,0,-0.203591,4.372576,2.192335 C,0,2.163312,-3.821251,3.369313 H,0,2.031256,-4.370377,4.296461 C,0,-4.261503,-1.295223,1.898499 H,0,-4.144321,-2.362827,2.067942 H,0,-4.622228,2.521242,1.423535 H,0,-5.885318,1.382267,3.198543 O,0,1.271197,-4.47036,-2.32993 C,0,1.477761,-3.541733,-1.592787 O,0,2.493483,-2.734108,-1.563887 O,0,1.09285,3.527739,-1.553405 C,0,2.26932,3.038799,-1.7929 O,0,3.064939,3.358263,-2.63868 O,0,-3.857358,-1.205744,-2.278438 C,0,-4.61627,-0.387236,-2.619173 O,0,-5.398938,0.391146,-2.976537 H,0,-2.083774,7.158855,-0.184854 H,0,-5.65673,-1.075031,3.524213 H,0,-4.767494,-5.613093,-0.378669 H,0,4.051271,-2.979024,3.952983 H,0,7.271327,-1.453257,-1.384356 H,0,1.342376,4.529612,4.111593</p>
	<p>2CO₂-Al₃P₃:CO₂ E=-3932,00000887H; FreqIm=0 C,-4.465251135,2.784717537,3.0781412981 C,-2.6929344455,2.7924640055,0.9048231144 C,-3.6161776175,1.7203903548,1.0465227905 C,-2.6667019795,3.827291207,1.8430854517 C,-3.5512211182,3.8218951946,2.9236269459 P,-1.4930466261,-2.7551342321,-0.2864287749 P,-1.6386000221,2.8145238089,-0.6353639951 C,-1.4072920341,0.0771924124,-0.4317397932 C,-4.1064781542,-1.6357071098,-0.1481896291 C,-0.6958634512,-1.1235481965,-0.3927045986 C,-1.3744510787,5.5031687698,-0.6428189477 H,-2.4537719293,5.4225146909,-0.7681559315 C,-0.5972786637,4.3377378525,-0.5149373524 C,-0.6397398573,1.2682459949,-0.4539454432 C,-5.4951948805,-1.8465231609,-0.1191678687 H,-6.1614303278,-0.9934182576,0.002716671 C,0.812624651,4.4338840584,-0.4047727707 C,-3.3024620374,-2.7902661122,-0.3090387878 C,-3.8608885973,-4.0690483037,-0.4504447691 H,-3.221822459,-4.9364957961,-0.5945480703 C,-6.0614926561,-3.113838303,-0.2480167282 C,-0.7929029153,6.7653200418,-0.6078091847 H,-1.4159415861,7.6508536537,-0.6969475926 C,0.5896358954,6.8818077991,-0.4758508015 C,1.3648188336,5.7288796866,-0.3879323205 H,2.4456412252,5.8415270302,-0.3092407128 C,-5.2423776577,-4.2278425364,-0.4195805192</p>

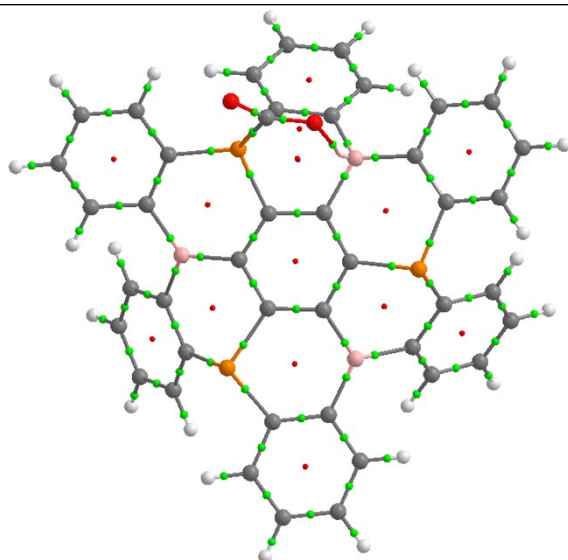
	<p> H,-5.6740959917,-5.2172809456,-0.5341791343 C,0.7564025806,1.2570523509,-0.4554532492 C,5.7039983672,-3.7410408221,-1.0004434806 C,4.0747685877,-1.5098205041,-0.696290678 C,3.4702061139,-2.7907319712,-0.6285536504 C,4.3345114116,-3.8875397779,-0.7858955986 H,3.924740193,-4.8955527437,-0.7482280614 C,5.4512207758,-1.3504683827,-0.9198292399 H,5.8866131985,-0.356896039,-0.9918950633 C,6.2649676098,-2.468039033,-1.0695771857 H,7.3282245038,-2.3409966751,-1.2482306976 P,3.1920874467,0.0603844887,-0.490531061 C,0.7086248277,-1.2305604649,-0.4301196974 C,0.5786120957,-3.8209398372,1.2012638315 C,4.5765909869,0.3887275,1.9334631308 H,4.9560700608,-0.6203503081,1.7905595832 C,3.7189538652,0.9727014971,0.9986288012 C,1.3734895416,-0.0107418088,-0.4661478668 C,1.0812390558,-4.4760394553,2.3322037512 H,2.1518332567,-4.6552668768,2.4132674252 C,3.1913085227,2.2785973577,1.1377162475 C,-0.8227346281,-3.6201616598,1.1758180684 C,-1.6724253112,-4.0419148983,2.2012619023 H,-2.7441000261,-3.865611792,2.1488842232 C,0.2500169762,-4.9106345226,3.3676553506 C,4.9387333804,1.1216734385,3.0626905118 H,5.6048169024,0.684081801,3.8004246132 C,4.4406053757,2.4109436441,3.2386406911 C,3.579721235,2.9713828646,2.2914154558 H,3.2023680932,3.978362076,2.4609259011 C,-1.1245174193,-4.6931973761,3.3052756952 H,-1.7710214017,-5.025695149,4.1118921412 C,-4.4792705478,1.7411856725,2.15071883 H,-5.1839686549,0.9233017174,2.2981491285 H,-1.9517498874,4.6395667241,1.7460266866 H,-3.5151606335,4.630815487,3.6483480405 O,-1.5205050021,-4.2876693967,-2.5258061895 C,-0.7597454196,-3.7798819089,-1.7415926765 O,0.5299650462,-3.8311329539,-1.7084352446 O,3.0612696957,2.4352784053,-1.76006494 C,3.6399496599,1.2916734581,-1.9037828832 O,4.4040583604,0.9278628186,-2.7614933092 O,-4.0257411076,0.91044954,-1.9401904337 C,-3.9308086849,1.8998206417,-2.5802048039 O,-3.9512974332,2.8055075812,-3.2865212734 H,1.0585026868,7.861795271,-0.4570207134 H,-5.1550877769,2.78190103,3.9174512869 H,-7.1411160474,-3.2323552105,-0.2212955305 H,0.6767717313,-5.4194506322,4.2279005741 H,6.3323019442,-4.6193395675,-1.1205870718 H,4.7231601779,2.9821415533,4.1190786434 Al,-3.3268451429,0.1717815877,-0.1148467127 Al,1.5264936334,-3.0241349478,-0.3693699955 Al,1.93950584,2.8300860649,-0.3301617524 </p>
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Table S3: Molecular graphs, energies (in Hartree) and Cartesian coordinates (in Å) of the transition states in vacuum. Level of theory: M06-2X/6-311++G*//M06-2X/6-31+G*

	<p>B₃N₃-NG/CO₂ E= -2042,29937279H; FreqIm=1</p> <p>C,5.9623354192,-0.2303782555,1.691468931 C,3.5597406496,-1.1133554794,0.5130405841 C,3.8941039819,0.2646442068,0.4807693589 C,4.4083211051,-2.016828099,1.1821903632 C,5.5908422559,-1.5789159135,1.753279387 C,1.4374887063,0.6802811914,-0.1028518887 C,2.9070808905,2.7539902412,-0.398100935 C,0.2960381477,1.513862906,-0.1270471282 C,3.3489394061,-3.5767597667,-1.0329416542 H,4.282923753,-3.0321074297,-1.1189006771 C,2.2143268391,-2.9443274719,-0.503601545 C,1.2554425508,-0.7188976668,-0.1372932748 C,4.0837303131,3.3715563868,-0.8647753201 H,5.0141594896,2.8114868504,-0.8205070048 C,0.9737729996,-3.6173479636,-0.5067406815 C,1.6950097156,3.4742471563,-0.5057320922 C,1.6822374188,4.7386598711,-1.1180953733 H,0.7426692314,5.2590523274,-1.2692594678 C,4.0799846415,4.6393906106,-1.4234224166 B,2.8251271635,1.262898486,-0.0003640523 C,3.2877868127,-4.8958389027,-1.4639093751 H,4.1814099835,-5.3633867567,-1.8673333563 C,2.0884568514,-5.6044107401,-1.3969691757 C,0.9500208566,-4.9489512491,-0.9436272083 H,-0.0071521517,-5.4673934867,-0.9522860479 C,2.8627846041,5.314114161,-1.5611990251 H,2.8288813465,6.2873487535,-2.0424507356 B,-0.3521297317,-2.7996750139,-0.2539935852 C,-0.0294946518,-1.2692779607,-0.2391207819 C,-5.9649177516,1.1029434447,-0.9635819399 C,-3.6066656178,-0.2857568213,-0.4494896249 C,-3.5803121843,1.1199329313,-0.4073921638 C,-4.7877859201,1.7856845837,-0.6928102978 H,-4.7878774057,2.870757428,-0.7285152565 C,-4.7880139137,-0.9836304061,-0.7113711176 H,-4.7832955308,-2.0691230982,-0.7348844194 C,-5.9656093299,-0.292800888,-0.9562222782 H,-6.8765468229,-0.8450880033,-1.1653132119 C,-1.0109231679,0.9837113674,-0.175692235 C,-1.9451170455,3.293560229,0.355241277 C,-3.4760552691,-2.0437490551,1.817726376 H,-4.247883914,-1.282598032,1.798727019 C,-2.479768477,-2.0966249301,0.8502676659 C,-1.0990231266,-0.4116084095,-0.2383237745 C,-2.9218741659,4.1472038297,0.9125404572 H,-3.9550191529,3.8138869566,0.9249501401 C,-1.4460033711,-3.0416994528,0.8819367165 C,-0.5917308622,3.7182444901,0.4071388461 C,-0.2674646158,4.9349372419,1.0386171512 H,0.7701171551,5.2275849703,1.1498294254 C,-2.6046821432,5.3618840192,1.4921191185</p>
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	<p>B,-2.2354524263,1.852781708,-0.1082461223 C,-3.4536891565,-2.993336859,2.84175093 H,-4.2215674188,-2.9613796563,3.6087089406 C,-2.4542963856,-3.9619994167,2.8883932544 C,-1.4534076067,-3.9764994411,1.915520029 H,-0.6560418537,-4.7148833753,1.9621451887 C,-1.2600163176,5.744398433,1.5617488068 H,-0.9800481571,6.6694439638,2.0576764234 C,5.107474896,0.6668768438,1.0764758531 H,5.3512551969,1.7262272409,1.0847548768 H,4.1239273276,-3.0583560521,1.2774343097 H,6.2201082436,-2.2942478933,2.2754100873 O,-1.2948075672,-2.933731777,-1.6122092246 C,-2.2045492152,-2.1210039851,-1.8228772757 O,-2.9563904246,-1.7830077163,-2.663459825 H,5.0008560066,5.0886558867,-1.7822439305 H,-6.8763353196,1.6494905056,-1.1863331737 H,-2.4475985948,-4.6952324259,3.6897057208 H,2.038444721,-6.6371868274,-1.7286364716 H,6.8867924788,0.1077192841,2.1492398419 H,-3.3792769711,5.9911801129,1.9191212819 N,-2.4065414914,-1.1034903615,-0.2703153757 N,0.4607226302,2.8987292914,-0.0790533153 N,2.3437014405,-1.580218871,-0.0462735249</p>
	<p>Al₃N₃-NG/CO₂ E = -2694,9166646H; FreqIm=1 C,6.0215346065,-0.5936176153,2.2248055679 C,3.6450921237,-1.0608160718,0.7649912532 C,4.2109051221,0.2418008054,0.7966337549 C,4.2673047485,-2.0893433851,1.5013595556 C,5.4334655413,-1.8612514449,2.2137177697 C,1.3713602018,0.7534189244,-0.0248609967 C,2.7012705862,3.3945279577,-0.5076764138 C,0.1809341094,1.4971760423,-0.0825221551 C,3.8305405488,-2.8984732439,-1.3601005571 H,4.546153066,-2.0816236811,-1.3893486009 C,2.6186114088,-2.7210911758,-0.670141612 C,1.2998264576,-0.653084715,-0.0804733324 C,3.6263969466,4.2718232512,-1.1049586422 H,4.6898873451,4.0657998697,-0.9989280724 C,1.6613066115,-3.7668264168,-0.6583231032 C,1.3204916788,3.6785999953,-0.6619055306 C,0.9305810936,4.7902983073,-1.4313362016 H,-0.1276689554,4.9918554916,-1.5703614848 C,3.2351287782,5.3902964125,-1.8287781918 C,4.1349635552,-4.0991877841,-1.9857348326 H,5.081348414,-4.2042789001,-2.5089156032 C,3.2246942578,-5.1549486924,-1.9504829943 C,2.0051807291,-4.9653928079,-1.3101653626 H,1.284479068,-5.7813159623,-1.3214952907 C,1.8712141083,5.6345860081,-2.0019099878 H,1.5366521523,6.4821047639,-2.5935758354 C,0.0699151318,-1.3110612941,-0.2063658659 C,-6.3456453849,-0.074634386,-1.1844891299 C,-3.6861288625,-0.7672983925,-0.6206095221 C,-4.0643265712,0.5855871309,-0.5668058385</p>

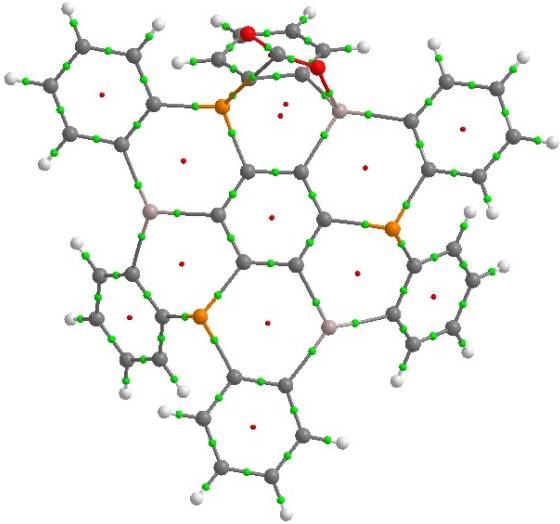
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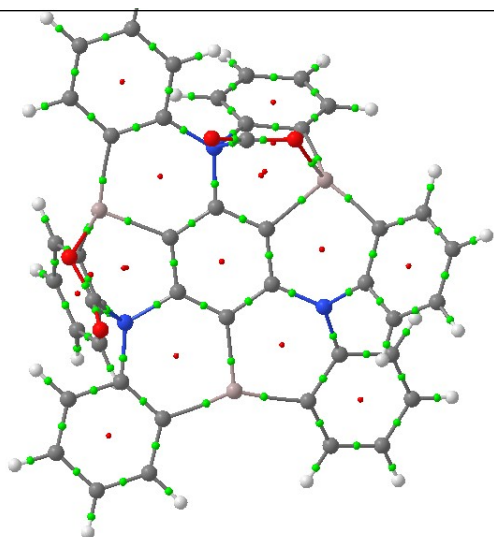
B₃P₃-NG/CO₂

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 C,0,4.049659,-3.134395,-0.963633
 C,0,3.973152,-4.113474,-1.953671
 P,0,-2.523093,-1.564492,0.469053
 P,0,2.960854,-1.542548,1.122132
 C,0,0.27371,-1.415435,0.610924
 C,0,-0.921952,-3.843417,0.308666
 C,0,-0.938188,-0.725243,0.529052
 C,0,5.621618,-0.852336,1.069744
 H,0,5.774344,-1.900222,1.321195
 C,0,4.325644,-0.37515,0.825076
 C,0,1.447698,-0.620471,0.742433
 C,0,-0.780805,-5.238484,0.411595
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 C,0,4.106287,1.000793,0.569756
 C,0,-2.241661,-3.334703,0.378545
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 B,0,0.344169,-2.91678,0.19741
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 H,0,7.71388,-0.382765,1.214666
 C,0,6.517974,1.368199,0.811575
 C,0,5.2326,1.848591,0.591776
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 H,0,-4.027717,-6.207931,0.708254
 B,0,2.677919,1.59406,0.346025
 C,0,1.40132,0.780408,0.727987
 C,0,-4.157057,4.800947,0.485568
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 C,0,-1.803079,5.138776,0.872295
 H,0,-0.985441,5.80049,1.153025
 C,0,-3.088324,5.656112,0.757233
 H,0,-3.260061,6.717953,0.909605
 P,0,0.128952,3.192587,1.068882
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 C,0,-3.237582,0.590292,-0.982851
 C,0,1.032117,4.829673,-1.073895
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 C,0,1.263361,3.700515,-0.288405
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 C,0,-3.838314,1.242305,-2.06751
 H,0,-3.790004,2.326467,-2.128297
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 C,0,-3.298362,-0.821042,-0.982658
 C,0,-3.952984,-1.546526,-1.974715
 H,0,-3.982434,-2.633037,-1.93779
 C,0,-4.483944,0.530561,-3.080057

	<p>B,0,-2.413348,1.364933,0.140725 C,0,1.941958,5.192373,-2.06676 H,0,1.739575,6.059417,-2.689662 C,0,3.089072,4.431364,-2.275301 C,0,3.329384,3.318519,-1.472812 H,0,4.214591,2.717081,-1.662323 C,0,-4.547526,-0.860276,-3.033309 H,0,-5.048876,-1.412911,-3.822455 C,0,1.625468,-4.379813,-1.505322 H,0,0.676965,-4.85197,-1.747818 H,0,4.997976,-2.637488,-0.779935 H,0,4.863333,-4.3748,-2.519228 O,0,-4.20683,-1.523722,2.747692 C,0,-3.703536,-0.695687,2.045937 O,0,-3.609286,0.501507,1.834918 H,0,-1.729928,-7.155256,0.6367 H,0,2.693167,-5.486969,-3.012865 H,0,7.361169,2.05255,0.824607 H,0,3.789293,4.698518,-3.061234 H,0,-5.169344,5.190847,0.43132 H,0,-4.93745,1.065025,-3.909834</p>
	<p>Al₃P₃-NG/CO₂ E= -3554,72945685H; FreqIm=1 C,3.4988775333,-4.5221274188,-2.4438504888 C,3.1776005575,-2.6624588953,-0.3563066748 C,2.1514410563,-3.6089626181,-0.6201305187 C,4.3322737469,-2.6581710102,-1.1445554998 C,4.4894853186,-3.5826356867,-2.1797449781 P,-2.5793855529,-1.649169367,0.6573712821 P,3.0128145234,-1.5836413976,1.1642364605 C,0.2906449614,-1.4290911329,0.754535217 C,-1.2654473083,-4.2210178908,0.2630700758 C,-0.944131116,-0.7807583267,0.677027097 C,5.6835742851,-1.1861635322,1.446157646 H,5.6186066107,-2.2202110493,1.7811965369 C,4.5160648713,-0.5078018404,1.0574075746 C,1.4551572198,-0.6140500599,0.8390060252 C,-1.3861503028,-5.6187112287,0.1655275066 H,-0.4994737131,-6.2192215411,-0.0325276104 C,4.5968643492,0.8489045407,0.6633882613 C,-2.4398765432,-3.478011378,0.5305714296 C,-3.6652353308,-4.1375229866,0.7134017416 H,-4.5614456832,-3.5624173679,0.9405090757 C,-2.6084411832,-6.2684117287,0.3193494659 Al,0.4274809512,-3.2709220029,0.2085667914 C,6.9266482055,-0.5631694129,1.3982033298 H,7.8169705583,-1.1126843051,1.6910446545 C,7.023021604,0.7662905063,0.9883365105 C,5.8655590243,1.4572357861,0.6418561219 H,5.9513257263,2.5034653795,0.3512580323 C,-3.7522588815,-5.5217666681,0.5978863404 H,-4.7102227084,-6.0154327188,0.7338284086 Al,2.9378446497,1.808227564,0.3919444285 C,1.373562944,0.7817899998,0.8568178956 C,-3.8750472323,5.5554166454,0.5773889843 C,-1.5442066744,4.0010137102,0.8152232788</p>

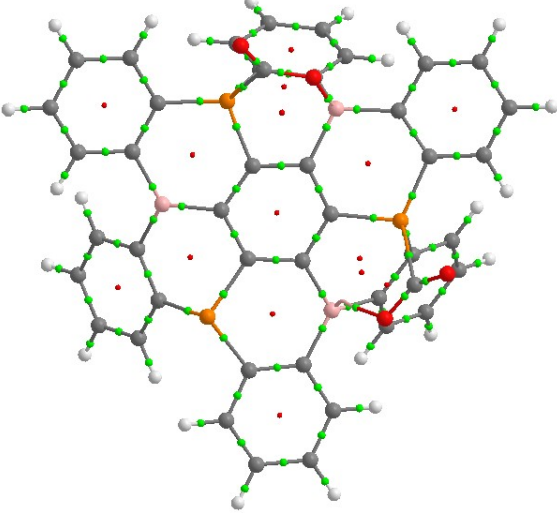
	<p> C,-2.7573275057,3.3760731858,0.445003025 C,-3.9037062148,4.1850645841,0.3357240967 H,-4.8530021357,3.7284878628,0.055948992 C,-1.530143035,5.3780523141,1.1010889439 H,-0.6036271042,5.8514632407,1.4231291027 C,-2.6772254032,6.1528699883,0.9687822654 H,-2.6377263375,7.2175359146,1.1818634408 P,0.1253462912,3.233664292,1.0542785493 C,-1.0880415582,0.6332138168,0.7214455467 C,-3.6168875929,0.2684608773,-1.0846729957 C,0.5558234139,4.782950143,-1.3238550338 H,-0.478153676,5.1042468085,-1.2406374063 C,1.0801913459,3.8384833714,-0.436622537 C,0.0841653477,1.3878898464,0.7970156604 C,-4.2629003219,0.6810441352,-2.2575672792 H,-4.4690991332,1.7394006986,-2.4116770502 C,2.4280425531,3.4138019047,-0.5778447609 C,-3.3486663937,-1.1163124149,-0.9438609802 C,-3.7300183838,-2.0318117423,-1.9285182954 H,-3.5172972006,-3.0916490359,-1.8142404602 C,-4.6544996761,-0.2276920243,-3.2430980286 Al,-2.8053609589,1.4412113579,0.2748972321 C,1.350869908,5.3216725942,-2.3382037483 H,0.9224223548,6.0514966476,-3.0201144944 C,2.6760163256,4.9251121892,-2.482614861 C,3.1961781499,3.9652245819,-1.6131406829 H,4.2270535543,3.6407173039,-1.7506936358 C,-4.3837411056,-1.5828016259,-3.0772299332 H,-4.6742505629,-2.2967760242,-3.843102001 C,2.33538049,-4.5163531887,-1.6733432195 H,1.5533216963,-5.2386662557,-1.9045835004 H,5.1194178002,-1.9313013804,-0.968151692 H,5.3929019666,-3.5579543146,-2.7833148819 O,-4.6615371145,-1.0535115382,3.0446632724 C,-4.1941851168,-0.2392884468,2.3666337997 O,-3.9423911292,0.8246740592,1.8873059988 H,-2.6686586123,-7.3496866673,0.23405227 H,3.6244629782,-5.2441724573,-3.2456338099 H,7.9893271767,1.2616372175,0.9558969035 H,3.294981607,5.3492325831,-3.2681961963 H,-4.7784753014,6.1508350658,0.4779264709 H,-5.1636818517,0.1211629642,-4.1374014877 </p>
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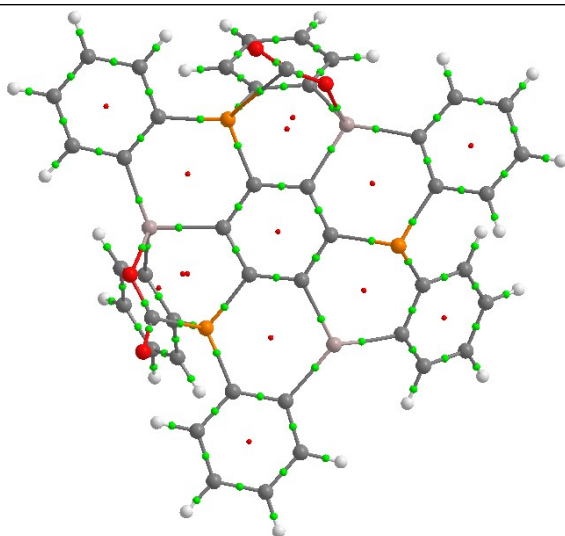
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 C, 1.17572800,-4.66788400, 3.04145400

	<p>Al, 2.25143700,-2.21822600,-0.36380900 C, 3.84807200, 1.84191100, 3.21635700 H, 4.51286500, 1.37280200, 3.93545600 C, 3.21200400, 3.04139800, 3.51715400 C, 2.33522100, 3.59935500, 2.58854100 H, 1.81544400, 4.51895700, 2.84832400 C, -0.20747300,-4.60042100, 2.90702100 H, -0.85700700,-5.03241200, 3.66249700 C, -5.46500600, 0.55288200, 1.23946400 H, -6.05720200,-0.35974200, 1.19653000 H, -3.36444100, 3.77033500, 1.47649800 H, -5.52743600, 3.64057100, 2.61859000 O, -0.52980700,-2.95560200,-2.89790800 C, 0.28353200,-2.99877200,-2.05444600 O, 1.49707000,-3.13430900,-1.86266200 O, 1.98445000, 3.23311700,-1.42029400 C, 2.45238600, 2.09687200,-1.67814300 O, 2.81108000, 1.53140100,-2.65643900 H, -2.22949600, 6.91962300,-2.16857600 H, -6.92556200, 1.57574300, 2.44831800 H, -5.05449800,-5.59642400,-1.25811900 H, 1.61967300,-5.16221200, 3.90083100 H, 7.24301600,-1.38262600,-1.21941100 H, 3.38177200, 3.52720800, 4.47392300</p>
	<p>1CO₂-B₃P₃-NG/CO₂ E= -3090,63699532H; FreqIm=1 C,0,-2.77962,5.068896,1.993126 C,0,-0.893069,4.000541,0.210768 C,0,-2.152658,3.354467,0.361067 C,0,-0.614671,5.169044,0.92151 C,0,-1.547913,5.694647,1.813802 P,0,-2.895591,-1.150593,-0.351733 P,0,0.260881,3.343541,-1.065994 C,0,-1.21661,1.071305,-0.624867 C,0,-3.912328,1.40392,-0.503337 C,0,-1.336519,-0.317943,-0.564656 C,0,2.360257,5.109185,-0.829812 H,0,1.611046,5.84794,-1.108369 C,0,1.985749,3.770034,-0.639352 C,0,0.104158,1.580192,-0.6874 C,0,-4.978298,2.282352,-0.754314 H,0,-4.783366,3.351039,-0.780037 C,0,2.970589,2.791793,-0.363345 C,0,-4.231248,0.020691,-0.526892 C,0,-5.52402,-0.45214,-0.760862 H,0,-5.719387,-1.521002,-0.793837 C,0,-6.272882,1.823414,-0.998518 B,0,-2.445491,1.971017,-0.303161 C,0,3.688733,5.502375,-0.712535 H,0,3.958537,6.545146,-0.853796 C,0,4.673042,4.547673,-0.456988 C,0,4.309638,3.216134,-0.293276 H,0,5.082132,2.469205,-0.12545 C,0,-6.552288,0.459127,-0.991179 H,0,-7.55908,0.102135,-1.183591 B,0,2.628093,1.277946,-0.156433</p>

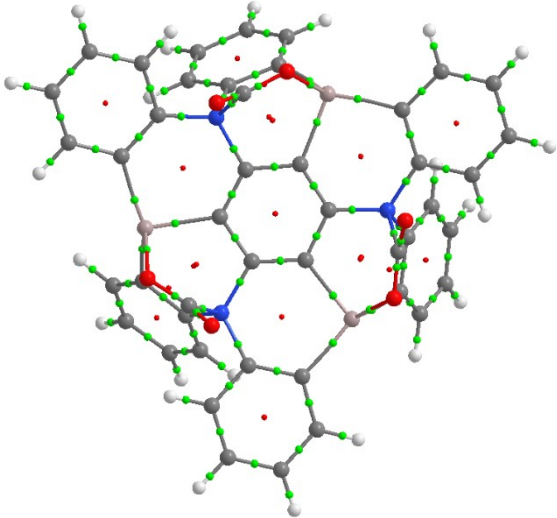
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C,0,-0.281808,-1.236002,-0.562037
C,0,-1.508671,-2.890033,1.05828
C,0,3.927993,-1.821045,1.850105
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C,0,3.325189,-1.022012,0.88138
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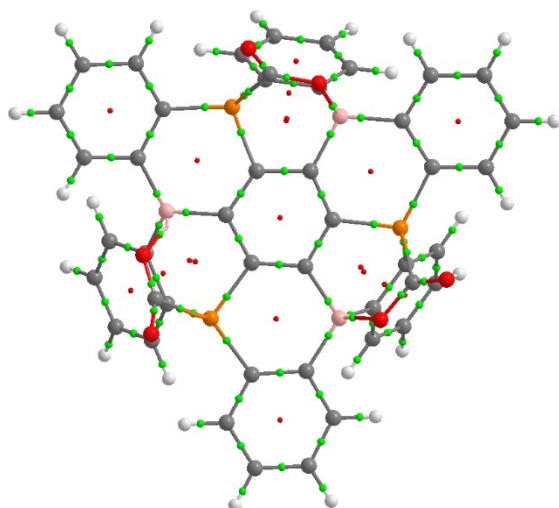
1CO₂-Al₃P₃-NG/CO₂

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 C,-3.07363200,-4.08420000, 1.18248900
 C,-2.90003500,-5.05102900, 2.17563400
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 C, 0.32115800,-1.56132000,-0.68698100
 C, 2.69834200,-3.71620400,-0.37763300
 C, 1.29277100,-0.55925200,-0.58189200
 C,-4.87730600,-3.05081700,-1.29332700
 H,-4.47941000,-4.03339100,-1.54465700
 C,-3.99409500,-2.00207100,-0.97646800
 C,-1.04690200,-1.17807300,-0.71432400
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 H, 2.61998400,-5.86441700,-0.16749300
 C,-4.50705700,-0.70885900,-0.71042100
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 H, 5.59480900,-2.01321600,-1.06672500
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 H,-6.33148300, 0.43185400,-0.53612000
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 H, 4.04017000, 2.91983600, 2.40909300
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 H, 4.62594500,-1.94917300, 1.67379000
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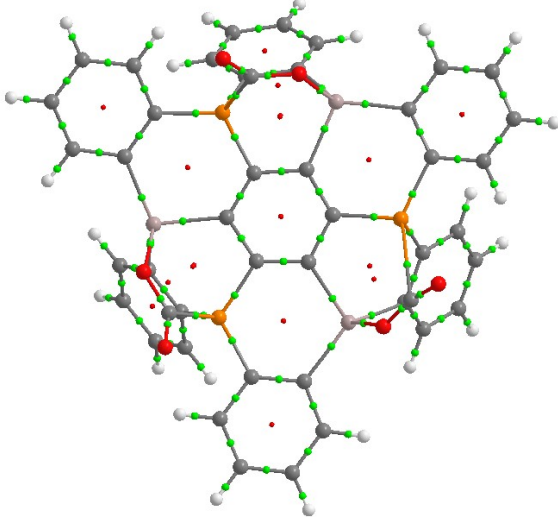
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2CO₂-B₃P₃-NG/CO₂

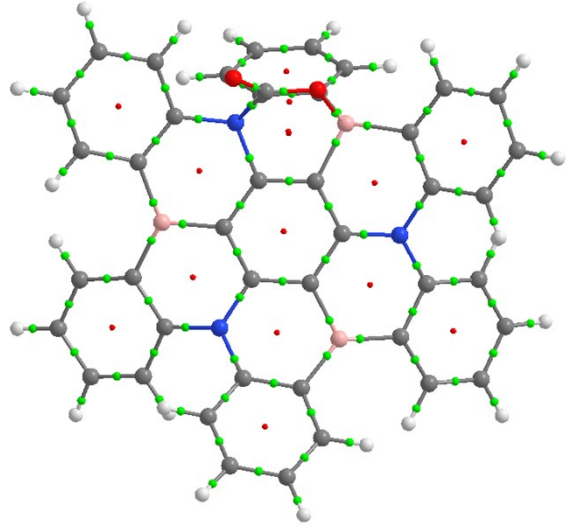
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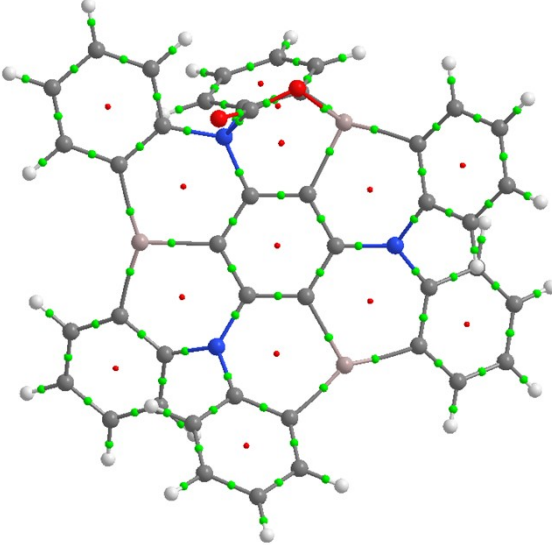
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	<p>B,0,2.863677,-1.044055,-0.434829 C,0,1.976911,4.026663,3.211275 H,0,2.592363,4.27504,4.070556 C,0,0.622418,4.356282,3.195782 C,0,-0.18179,4.041749,2.095977 H,0,-1.235596,4.311311,2.108793 C,0,2.829212,-3.57061,3.264741 H,0,2.802432,-4.198194,4.150171 C,0,-3.813378,-2.254116,1.917745 H,0,-3.50445,-3.293508,2.003957 H,0,-4.90451,1.456831,1.688481 H,0,-5.809239,0.009661,3.482217 O,0,2.172125,-4.008125,-2.478877 C,0,2.166492,-3.107509,-1.681648 O,0,2.991572,-2.109245,-1.575278 O,0,0.314731,3.627637,-1.562041 C,0,1.579351,3.40304,-1.757156 O,0,2.306679,3.870724,-2.59403 O,0,-3.339586,-1.593724,-1.922336 C,0,-3.815614,-0.541376,-2.285484 O,0,-4.470151,0.058669,-3.066918 H,0,-3.663574,6.48304,-0.494647 H,0,-5.111086,-2.368861,3.633419 H,0,-3.56459,-6.482066,-0.738071 H,0,4.495374,-2.400755,3.950188 H,0,7.418707,0.096953,-1.115125 H,0,0.185808,4.865097,4.050926</p>
	<p>2CO₂-Al₃P₃-NG/CO₂ E=-3931,99895508H; FreqIm=1 C,3.9579403098,3.0947268097,3.2849185195 C,3.4935365491,1.5531440544,1.0449959852 C,2.7644819667,2.7598485376,1.1738854569 C,4.4237404961,1.1154891222,1.990233945 C,4.6550159936,1.8998787509,3.1192664805 P,-2.0684190214,2.5009857635,-0.6038971861 P,3.1346071285,0.5619254978,-0.4445173051 C,0.5414459175,1.3545863933,-0.4307238771 C,0.0771026847,4.4961845036,-0.4045250763 C,-0.8367980394,1.1391616686,-0.4406925698 C,5.5942395063,-0.4725056677,-0.8376387352 H,5.867907943,0.5778693168,-0.900158756 C,4.2570557975,-0.8487012167,-0.6365886515 C,1.3520376081,0.2011562573,-0.438239114 C,0.4104768087,5.8636772195,-0.4020722256 H,1.4581441702,6.1520799098,-0.3242000111 C,3.8613467733,-2.2096962723,-0.5827169616 C,-1.2996553812,4.1747596291,-0.5133479 C,-2.2575549612,5.1949685528,-0.6509138316 H,-3.3095436511,4.938186244,-0.7714060356 C,-0.5422096763,6.8742302008,-0.5031364333 Al,1.4540856399,3.097858484,-0.3068136821 C,6.5770424989,-1.4462401153,-0.9769930133 H,7.6093794514,-1.1515954619,-1.1383039424 C,6.2235924925,-2.792209597,-0.9197989247 C,4.891262078,-3.1546365245,-0.7283487058 H,4.6459884804,-4.2150490826,-0.7003000986</p>

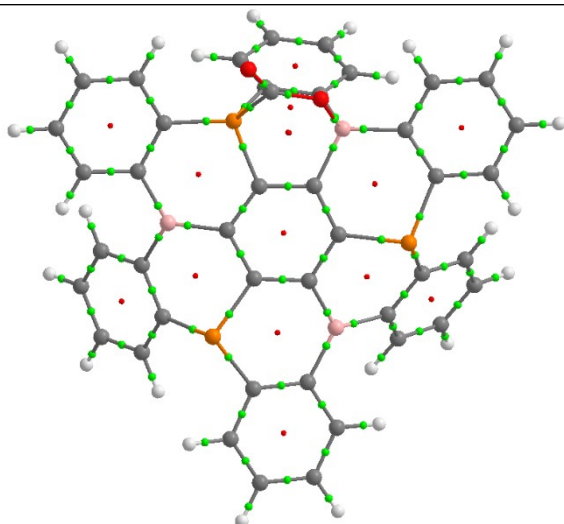
<p> C,-1.887610267,6.535034286,-0.6316933393 H,-2.6454184709,7.3071751491,-0.7294786799 Al,1.9742594635,-2.7528570988,-0.3630437806 C,0.8877635748,-1.1085494044,-0.4193998723 C,-5.5114657903,-4.0245726428,-0.4498881039 C,-2.8365176737,-3.2721437565,-0.4119601096 C,-3.8170908752,-2.2583430492,-0.2760932451 C,-5.1553987146,-2.6854680712,-0.2966148436 H,-5.9511115295,-1.9486747959,-0.1954435778 C,-3.1831121973,-4.6212535638,-0.5767404051 H,-2.4117657393,-5.3770538417,-0.7016028426 C,-4.5226888096,-4.9951227979,-0.595264937 H,-4.7894353217,-6.0389630701,-0.72839259 P,-1.0540187048,-2.9625269221,-0.3405112072 C,-1.4087835056,-0.1559186425,-0.4354722903 C,-3.8496053693,1.0902735357,1.0439428535 C,-1.0751603406,-4.3097869173,2.1218459844 H,-2.1600014307,-4.3047088488,2.0481433176 C,-0.2838944184,-3.7393241243,1.1221505444 C,-0.5160379225,-1.2273761596,-0.4033474043 C,-4.7030710964,0.9590799894,2.1475665417 H,-5.266848173,0.0369430363,2.2843098522 C,1.1311575286,-3.7150339237,1.1754144984 C,-3.1160224457,2.3012697127,0.9203866931 C,-3.2574034546,3.3197049044,1.8658899659 H,-2.6855709748,4.2392410299,1.7745444201 C,-4.856836017,1.9807387627,3.0869364774 Al,-3.3333683901,-0.35092207,-0.1847762297 C,-0.4521732262,-4.8863699619,3.2276569921 H,-1.0530007962,-5.3326534753,4.0144137107 C,0.9378863302,-4.8835048306,3.3172060368 C,1.7092715661,-4.3029080063,2.3072400685 H,2.7929386598,-4.3112602807,2.409594266 C,-4.1274845583,3.1571249838,2.9455768666 H,-4.2257863959,3.9528462406,3.678955505 C,3.0279865639,3.5088594955,2.3276956669 H,2.4947465133,4.4440572705,2.4894736425 H,4.9591945569,0.1786087476,1.8555241361 H,5.3748569334,1.5752182986,3.8647849344 O,-4.0725553313,2.3465304913,-3.2261957073 C,-3.9364176055,1.4657569076,-2.4948092103 O,-4.0211730078,0.4107604211,-1.9433009141 O,1.1410742772,-3.6819435948,-1.733286018 C,-0.1399066559,-3.8353330223,-1.7929287798 O,-0.7948266503,-4.4457691924,-2.5988574878 O,2.6347126605,2.8819840768,-1.7256428391 C,3.3934212761,1.8465582501,-1.8575484732 O,4.2168416256,1.6105529197,-2.7046986311 H,-6.5595169828,-4.3105049577,-0.4626034937 H,-5.5352535159,1.8550897389,3.9262195074 H,-0.2381340312,7.9172985309,-0.4958349833 H,4.1384581667,3.7063320577,4.1650235362 H,6.9847346172,-3.5594842507,-1.0317612272 H,1.4235185127,-5.3339895414,4.1787498549 </p>

Table S4: Molecular graphs, energies (in Hartree) and Cartesian coordinates (in Å) of the adducts in vacuum. Level of theory: M06-2X/6-311++G*//M06-2X/6-31+G*

	<p>1CO₂-B₃N₃-NG E= -2042,3012114H; FreqIm=0</p> <p>C,-2.6745154959,-5.303445567,1.6179382291 C,-2.4464254636,-2.7385933456,0.4715635423 C,-1.3452977196,-3.6323865066,0.4219524133 C,-3.6235009255,-3.1263659827,1.1418291643 C,-3.7325398368,-4.3894241111,1.6970407287 C,0.082075933,-1.588748845,-0.1530044136 C,1.3249943852,-3.8026588898,-0.4684194611 C,1.3252429389,-0.9143874985,-0.171712948 C,-4.5913550295,-1.4607854171,-1.0406980901 H,-4.5018509748,-2.5365696378,-1.1465223471 C,-3.5294859582,-0.7177289874,-0.5053243588 C,-1.1041621569,-0.8253488486,-0.1721855263 C,1.3780152959,-5.1249652667,-0.9502349008 H,0.4736733642,-5.7265531356,-0.9108028629 C,-3.6011163221,0.6917051854,-0.4831877267 C,2.4949763543,-3.0151522491,-0.5703674127 C,3.6414824736,-3.537693819,-1.1912403555 H,4.5137344321,-2.9095977672,-1.336754322 C,2.5241581779,-5.6581012894,-1.5178410729 B,0.0131864812,-3.0931567767,-0.060755088 C,-5.7590552205,-0.8309245775,-1.4528645123 H,-6.5686522136,-1.4292387327,-1.8608365487 C,-5.8805206288,0.5550646922,-1.3617236094 C,-4.7951954817,1.2928231815,-0.903551526 H,-4.8503702497,2.3798837002,-0.8956900743 C,3.6549652134,-4.8459973916,-1.6491895629 H,4.5478441417,-5.2269276269,-2.1365829863 B,-2.2881413521,1.5380954158,-0.229081769 C,-1.0497462842,0.572529685,-0.2613034726 C,3.6375169357,4.9492216369,-0.835087069 C,1.3712286445,3.3991574681,-0.4062588385 C,2.6255294452,2.767516931,-0.3715440829 C,3.7469079317,3.583385249,-0.6161610847 H,4.7272513348,3.1197060582,-0.6612452685 C,1.2466464461,4.7741108253,-0.6077537228 H,0.2647884366,5.2367937213,-0.6173215193 C,2.3784249096,5.5502155054,-0.8112697846 H,2.2728720982,6.618083146,-0.9748618662 C,1.4075767717,0.4937310047,-0.205376726 C,3.8888757149,0.3423584028,0.34270322 C,-0.1967929486,3.8948438724,1.9383395381 H,0.8186204405,4.2721814219,1.8989463551 C,-0.718658694,3.0838961416,0.9401836749 C,0.1817184345,1.1634016129,-0.2624441026 C,5.0759920463,0.8498760664,0.9153138998 H,5.2161513997,1.9257080398,0.9498595999 C,-2.0087613089,2.5444929884,0.9871418816 C,3.694403115,-1.0642365845,0.3687675692 C,4.6550191498,-1.8884237278,0.9878223064 H,4.4764205159,-2.9533981714,1.0793571218 C,6.036627199,0.0339888523,1.4831732653</p>
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	<p>B,2.7143244526,1.2288554227,-0.1134034552 C,-1.0202845725,4.2063383916,3.0236897671 H,-0.6311661092,4.8351924885,3.818521377 C,-2.3191960889,3.7099606644,3.0922627996 C,-2.8045032696,2.8780715811,2.0806967553 H,-3.8106005307,2.469725257,2.1437071026 C,5.8086802286,-1.3466019823,1.5251320029 H,6.5237439272,-2.0039481611,2.0115581126 C,-1.5005802212,-4.9088254332,1.0020574211 H,-0.6485386561,-5.5838681286,0.9970421068 H,-4.4415018886,-2.423902856,1.2510181953 H,-4.6460149493,-4.657459568,2.2205292865 H,4.5245966521,5.5451709554,-1.0273589072 H,-2.949271477,3.9601738023,3.9409621606 H,6.9342076722,0.4578763026,1.9224904498 H,-2.764112787,-6.2893533759,2.0633780275 H,2.534651864,-6.6784332984,-1.8885616447 H,-6.7928032558,1.0510309609,-1.6795261408 O,-0.2992788722,3.5327430805,-2.5327624409 C,-0.8628317027,2.961898988,-1.6608895872 O,-2.0151815117,2.4921909807,-1.4922536976 N,2.5052261043,-1.6574142214,-0.1286941666 N,-2.3490101202,-1.4332404153,-0.070218423 N,0.1040522156,2.6576855135,-0.2573635976</p>
	<p>1CO₂-Al₃N₃-NG E= -2694,918696H; FreqIm=0 C,6.068486629,0.0529828875,2.1907208938 C,3.7490254584,-0.6709604117,0.7433917118 C,4.1763283178,0.6837731966,0.7632229402 C,4.4778274228,-1.6233754586,1.4847333426 C,5.6157557893,-1.2692478422,2.1909196114 C,1.2991952244,0.8940435615,-0.0586391524 C,2.3501152037,3.6534963821,-0.56656044 C,0.0380056386,1.5112148651,-0.119278162 C,4.1123585448,-2.5028468027,-1.3655615697 H,4.7403804277,-1.6173315088,-1.4069252884 C,2.8920419123,-2.4438541819,-0.670828314 C,1.3749524777,-0.5122697168,-0.1012855954 C,3.1785019762,4.6148529508,-1.1761719817 H,4.2577606526,4.5213344286,-1.070927502 C,2.0461650588,-3.5811563027,-0.6430736259 C,0.9473630877,3.7916846496,-0.7205303984 C,0.4428537312,4.8474781018,-1.5014437252 H,-0.6308407127,4.9364505765,-1.6397405192 C,2.6721454077,5.6783528334,-1.9116027839 C,4.5355870974,-3.6726487986,-1.9809776127 H,5.4853398325,-3.6857918749,-2.5084100432 C,3.7381579114,-4.8152019517,-1.9300849968 C,2.5083079314,-4.7446075848,-1.2851375696 H,1.8744661171,-5.6296753329,-1.2859413285 C,1.290146856,5.7780722588,-2.0841580331 H,0.8688631057,6.5794222527,-2.6846581743 C,0.2189212011,-1.2957627694,-0.2164778986 C,-6.3363297545,-0.7292987068,-1.0081767798 C,-3.6038689203,-1.1477359491,-0.5743130096 C,-4.1040522659,0.1611074609,-0.5117008312</p>

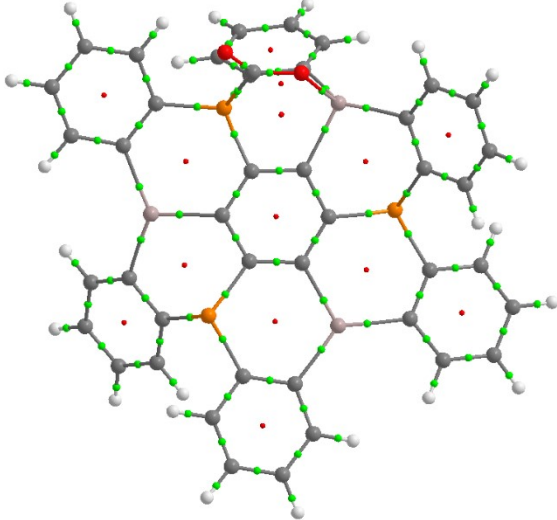
<p> C,-5.4862470966,0.3320304522,-0.7368401831 H,-5.903757426,1.3360565153,-0.6956087341 C,-4.4563094758,-2.2246610327,-0.847876822 H,-4.0569261223,-3.2360837983,-0.8769974998 C,-5.8085571846,-2.0207047035,-1.0657867974 H,-6.4494290411,-2.8702833047,-1.2804013517 C,-1.14924824,0.7522105015,-0.2036269404 C,-2.4957178926,3.3561025988,0.427595966 C,-3.190174586,-2.1661495694,1.9241164779 H,-3.9399894949,-1.4004427517,1.7624657729 C,-2.2040989787,-2.4389906638,0.9737203688 C,-0.9884424067,-0.628065418,-0.2427528272 C,-3.424239771,4.2208510693,1.0401467103 H,-4.48483222,3.9845419353,0.9737133016 C,-1.2051685276,-3.4036691481,1.1980310693 C,-1.1154019814,3.6752193512,0.5248153072 C,-0.733928808,4.815070966,1.2610420888 H,0.3216150997,5.0480811163,1.3639301412 C,-3.040353621,5.3623333599,1.7281486533 C,-3.2196128154,-2.896251776,3.1108571181 H,-3.9877520677,-2.6783303486,3.8467958758 C,-2.2762782832,-3.891010538,3.3446789116 C,-1.2821253804,-4.1237789125,2.3961933931 H,-0.5293090372,-4.8810753354,2.6036484827 C,-1.6769202543,5.6440738401,1.8470716337 H,-1.3441779471,6.5110107377,2.410992668 C,5.3370943914,1.0041773204,1.4952032884 H,5.6736269718,2.039225761,1.517962234 H,4.1394707019,-2.6549824194,1.4949154403 H,6.1484853605,-2.0301322432,2.7546077371 H,-7.3956070158,-0.5594699244,-1.1758240413 H,-2.3038314865,-4.4670634538,4.2653181338 H,-3.7818210054,6.012612242,2.1822348236 H,6.9634183956,0.3320549038,2.7386660055 H,3.3392136851,6.4072488403,-2.3620043166 H,4.0608006476,-5.7367430727,-2.4059246319 O,-2.2794343274,-1.9050616909,-2.7244661174 C,-1.7918627432,-2.4352153104,-1.7837386307 O,-1.050606254,-3.4230926689,-1.5797617532 N,-0.0434999833,2.9456116488,-0.0977376731 N,2.6327796388,-1.1795684027,-0.0029220625 N,-2.1942672855,-1.5944006199,-0.3048563096 Al,-2.8281976687,1.5715455995,-0.1862871084 Al,0.1935734561,-3.2243965585,-0.1690067471 Al,2.872833721,1.917604694,0.0824987805 </p>
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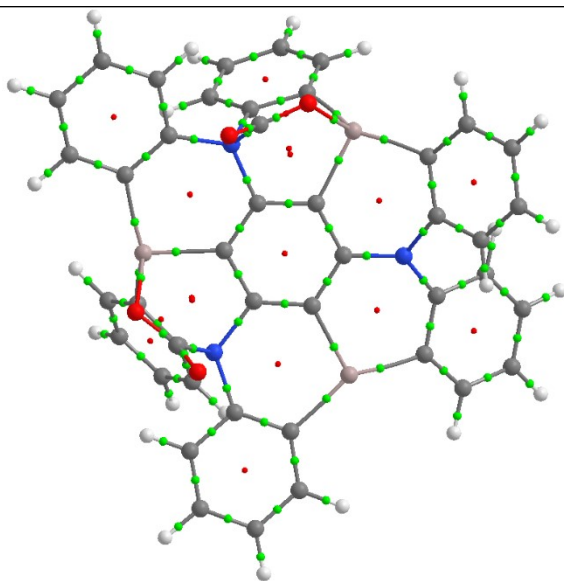
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	<p>B,0,-2.3843673723,1.7768548955,-0.4233802986 C,0,-3.01415127,-3.2574683307,2.8935789018 H,0,-3.6308270222,-3.320475645,3.7849518712 C,0,-1.8434884196,-4.0097713763,2.7912317874 C,0,-1.0387418929,-3.9416621022,1.6504709381 H,0,-0.1321137565,-4.5397424343,1.5962385979 C,0,-1.5681439086,5.3227275485,2.0113457896 H,0,-1.3415406409,6.1698686809,2.6528888378 C,0,4.2596123794,0.5378811753,1.6704946317 H,0,4.2524208234,1.5885311172,1.9486323497 H,0,4.1939676035,-3.2302895045,0.8220869958 H,0,5.4686231246,-2.4345142671,2.7727042476 H,0,5.7028830254,4.7620153588,-0.1276542563 H,0,5.4919815151,-0.0129868383,3.3487190566 H,0,1.2272032217,-7.329727471,-1.0984878066 H,0,-1.5534654625,-4.6595285225,3.6125098582 H,0,-7.0089365111,2.3580805436,-1.3022934787 H,0,-3.5220039399,4.989257141,2.8604143294 C,0,-2.6769064558,-2.6325857986,-2.0922197652 O,0,-1.5655615447,-3.2781515137,-1.9762626328 O,0,-3.5739031125,-2.7782803187,-2.884059608</p>
	<p>1CO₂-Al₃P₃-NG E= -3554,75305862H; FreqIm=0 C,5.7501554196,-3.6450447317,1.2417458916 C,3.018260623,-3.0261099375,0.9371992049 C,3.9949558605,-2.0597447418,0.5929811638 C,3.4304990934,-4.2608857871,1.4725568076 C,4.7764757687,-4.5757285314,1.6076451757 P,1.8224151119,2.6363142157,-1.0222503953 P,1.1805534686,-2.8190327284,0.9461425602 C,1.5100254111,-0.110479809,-0.0933816549 C,4.3793299529,1.3346661249,-0.3755435135 C,0.9138259912,1.1259125762,-0.4220319392 C,1.4126798182,-5.0192060267,-0.8700230125 H,2.4892638349,-4.9056533158,-0.786591071 C,0.5486592252,-4.1242929617,-0.2305655177 C,0.6694348063,-1.2236907921,0.1461986738 C,5.7853273497,1.4242988836,-0.3644277129 H,6.3723722034,0.5689288953,-0.0353648924 C,-0.8568484594,-4.254163474,-0.3827706938 C,3.6515622108,2.4676693728,-0.8115941699 C,4.3442071619,3.6079089721,-1.2579892385 H,3.7864641535,4.4623774925,-1.6386340542 C,6.4622776587,2.5719271239,-0.7615400886 C,0.9053406199,-6.0680155721,-1.6381631738 H,1.591860169,-6.7532073981,-2.1284592344 C,-0.4685082978,-6.2248909682,-1.7847396449 C,-1.3286343532,-5.3080486961,-1.1788753465 H,-2.3996454695,-5.4151404015,-1.3434949371 C,5.7318320635,3.669426009,-1.2177667368 H,6.2421978484,4.5672759869,-1.5549345105 C,-0.7281827145,-1.1461404498,-0.0036447615 C,-5.4181182238,4.0115615389,-0.8978852337 C,-3.9096789251,1.6984326014,-0.5543569302 C,-3.2474989245,2.9495345746,-0.5019085354 C,-4.0439317902,4.0931022708,-0.6771159525</p>

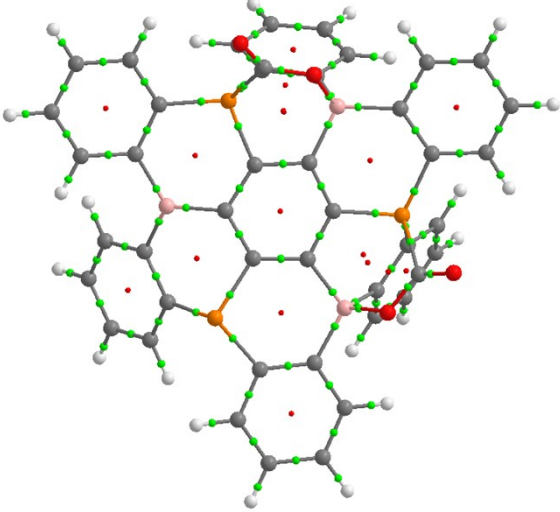
	<p> H,-3.5802410492,5.0776617771,-0.6492660596 C,-5.2881534254,1.6071340915,-0.7869792074 H,-5.7732900236,0.6362811782,-0.8452062428 C,-6.0396904906,2.7664503193,-0.9578482212 H,-7.1068341932,2.692940099,-1.1432241046 P,-3.0755456089,0.1123297094,-0.2853317123 C,-0.4887859039,1.2853695307,-0.4620485973 C,-0.0198484582,4.324596431,0.316120199 C,-4.5026404398,-0.0176639304,2.1225797034 H,-4.7996627137,1.0103185299,1.9290861226 C,-3.6725171609,-0.707659295,1.2348209387 C,-1.2499152626,0.1246950808,-0.2606844428 C,-0.3662218907,5.3975751863,1.1497704565 H,-1.4096898793,5.6975383153,1.2377484698 C,-3.2568953161,-2.0459340069,1.445145533 C,1.3468894972,3.9395513507,0.2367491822 C,2.2993627549,4.6289727197,0.9919706445 H,3.3439617684,4.334428786,0.9634899371 C,0.5938403137,6.0995957237,1.8793718066 C,-4.9481193136,-0.666133582,3.2728497764 H,-5.5916663858,-0.142598909,3.9735608896 C,-4.5620749947,-1.9823382464,3.515734052 C,-3.7293807618,-2.6519927122,2.6160171521 H,-3.4415876401,-3.6774625042,2.8377566949 C,1.923834215,5.7006304525,1.8055065696 H,2.6814830376,6.2179530959,2.3879458423 C,5.3516449615,-2.4050729963,0.7577081161 H,6.1229311937,-1.6814995417,0.4996255167 H,2.6827103202,-4.9893953529,1.7817001851 H,5.0657340702,-5.5431266966,2.0088159227 H,-6.0021364808,4.9177115783,-1.031431414 H,-4.9099775458,-2.4897413995,4.4116213625 H,0.3041856794,6.9377645936,2.5064809295 H,6.8049377035,-3.8811833055,1.3497139832 H,7.5476005485,2.6076264226,-0.7336794009 H,-0.867974846,-7.0407056153,-2.3810435004 O,-4.3003149429,-0.7812657718,-2.5356232369 C,-3.561694664,-1.1428402078,-1.6541475534 O,-3.0261722733,-2.2908560528,-1.4440042095 Al,-1.97700575,-2.7001099166,0.0464303054 Al,3.4147815687,-0.2957735135,0.0466973475 Al,-1.2997878842,3.0274512694,-0.3449062616 </p>
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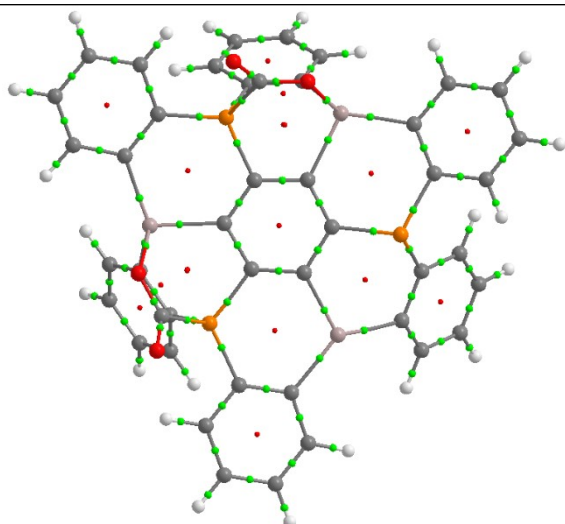
2CO₂-Al₃N₃-NG

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 C,3.4135008752,3.5472684599,1.3986961341
 C,3.5124069474,4.7718840902,2.0364721304
 N,-2.6263582616,0.9665498841,-0.2946891898
 N,2.3168869944,1.9295687155,-0.0137436121
 C,-0.1198578458,1.5232055863,-0.1579930014
 C,-2.3467207255,3.5524075506,-0.3829451526
 C,-1.1356710051,0.5820776739,-0.2159113567
 C,4.17396657,2.6675967094,-1.3566757841
 H,3.6170141093,3.5924384909,-1.4783961883
 C,3.603868935,1.6183536072,-0.6162098857
 C,1.2083291719,1.0329867618,-0.1071073731
 C,-3.0283757357,4.7740918201,-0.5665913695
 H,-2.4716924433,5.7041009667,-0.4708904866
 C,4.3008175672,0.3902497869,-0.4870184958
 C,-3.0995618784,2.3759551492,-0.5169849658
 C,-4.4658202103,2.4334313919,-0.8185064977
 H,-5.0402532786,1.5136388503,-0.9030006646
 C,-4.3810576104,4.8387797524,-0.8646054105
 Al,-0.4545156573,3.3647091435,-0.0441281116
 C,5.4379046543,2.5504038789,-1.9178057833
 H,5.8511674985,3.3807653366,-2.483455385
 C,6.1605081036,1.3680605262,-1.7648575685
 C,5.5760524627,0.3104972225,-1.0767263026
 H,6.1304202765,-0.6233036132,-1.0010537833
 C,-5.1026696688,3.650525221,-0.9935865787
 H,-6.1618853847,3.670266393,-1.2305618483
 Al,3.2128495991,-1.1484450494,0.0090970898
 C,1.4642433429,-0.3386398769,-0.1426462075
 C,-1.7514788322,-6.0963975898,-0.8887619691
 C,-0.253511797,-3.7745627148,-0.4612218882
 C,-1.6541362173,-3.6690031695,-0.488352972
 C,-2.3679526577,-4.8671090994,-0.7075916849
 H,-3.4551193751,-4.8272655524,-0.7377697274
 C,0.3783977813,-5.0115438798,-0.644428314
 H,1.4638259567,-5.0740419966,-0.6077554766
 C,-0.3581918462,-6.1640215009,-0.8572704753
 H,0.1554267087,-7.1097794785,-0.9998478955
 N,0.7553847097,-2.6808867172,-0.1901361741
 C,-0.9434209347,-0.7951536003,-0.2301786902
 C,-3.5202869621,-0.9661830819,1.1073519087
 C,0.7669630145,-3.7398209233,2.0818932747
 H,-0.2285928266,-4.1196805303,1.8847887756
 C,1.4621145978,-2.9849017891,1.135567337
 C,0.3742169899,-1.1936887162,-0.1955253094
 C,-4.171932343,-1.3864733079,2.2732910098
 H,-4.329935345,-2.4509199148,2.4330966741
 C,2.7337043203,-2.4449800845,1.405882483
 C,-3.3415039468,0.4189166116,0.9449886972
 C,-3.7380365462,1.3320481725,1.924294726
 H,-3.569795596,2.3967455342,1.8118644648
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	<p>Al,-2.4939530728,-1.9237717938,-0.2611392782 C,1.3633767521,-4.0152493179,3.3110641309 H,0.8176010805,-4.602790256,4.0432013519 C,2.6403450318,-3.5420239005,3.5924049652 C,3.300202667,-2.7588716596,2.6472055305 H,4.2839487943,-2.363919773,2.8912418096 C,-4.3709672159,0.8688166376,3.076034564 H,-4.6764572213,1.5831124033,3.8346228341 C,1.319490028,5.3479378367,1.2739939792 H,0.492678794,6.0556542158,1.2436650831 H,4.23465963,2.8406567123,1.4663874122 H,4.4102192394,5.0024148125,2.6032159815 O,-2.9156177283,0.9451597433,-2.7246756542 C,-3.0262139565,0.1929441573,-1.8182122452 O,-3.3310094167,-1.0158759186,-1.6755135775 O,2.9429981391,-2.4065085384,-1.363148778 C,1.7536222877,-2.7273266849,-1.6056936692 O,1.1369541226,-3.0259032042,-2.5724138758 H,7.1514015405,1.2654193732,-2.1975840664 H,2.5452432592,6.6607984559,2.4630099828 H,-4.8716247937,5.7981388009,-0.9983705443 H,-5.1085294021,-0.8514367574,4.1417753016 H,-2.3434940744,-6.991515229,-1.0551673353 H,3.1095753165,-3.7642483191,4.5466881847</p>
	<p>2CO₂-B₃P₃-NG E= -3090,65894931H; FreqIm=0 C,0,1.191862,5.532423,1.990475 C,0,1.915692,3.543629,0.137518 C,0,0.539281,3.874849,0.309093 C,0,2.890476,4.224524,0.87075 C,0,2.531923,5.202687,1.796203 P,0,-2.961706,0.943266,-0.373385 P,0,2.367633,2.341973,-1.188201 C,0,-0.245527,1.566041,-0.729859 C,0,-2.09013,3.54997,-0.505468 C,0,-1.245672,0.592223,-0.65829 C,0,5.099853,2.308943,-0.900511 H,0,4.99962,3.369813,-1.123948 C,0,3.951581,1.505641,-0.786592 C,0,1.089201,1.106092,-0.846237 C,0,-2.341383,4.913586,-0.724528 H,0,-1.501368,5.602078,-0.759882 C,0,4.075557,0.108688,-0.614694 C,0,-3.231599,2.703124,-0.511564 C,0,-4.5286,3.184781,-0.699803 H,0,-5.370947,2.497813,-0.719574 C,0,-3.631189,5.406867,-0.923745 B,0,-0.593918,3.036645,-0.357619 C,0,6.372139,1.76458,-0.775588 H,0,7.246935,2.403814,-0.854613 C,0,6.512478,0.389823,-0.586543 C,0,5.377718,-0.411547,-0.522454 H,0,5.493839,-1.487459,-0.401454 C,0,-4.727749,4.548814,-0.901011 H,0,-5.730844,4.93243,-1.058211 B,0,2.848978,-0.916609,-0.506247</p>

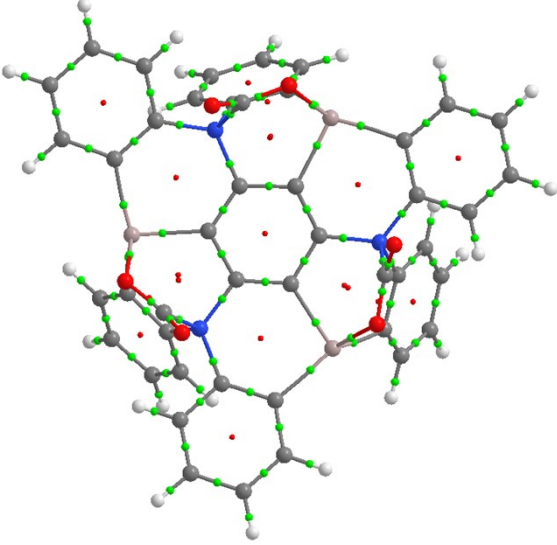
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	C,0,-0.638524,-3.903927,-0.500392
	C,0,-1.939176,-3.34213,-0.52404
	C,0,-2.995314,-4.258575,-0.635835
	H,0,-4.011615,-3.87182,-0.668994
	C,0,-0.409772,-5.285041,-0.590336
	H,0,0.60693,-5.671404,-0.603623
	C,0,-1.489281,-6.152776,-0.693712
	H,0,-1.321855,-7.222549,-0.769155
	P,0,0.793435,-2.832438,-0.421326
	C,0,-1.032708,-0.785909,-0.648391
	C,0,-2.966925,-1.308308,1.020351
	C,0,1.60038,-3.480454,2.231947
	H,0,0.82659,-4.243275,2.28269
	C,0,1.783231,-2.722972,1.079014
	C,0,0.303989,-1.140846,-0.677643
	C,0,-3.191969,-2.113303,2.138412
	H,0,-2.906352,-3.162727,2.104171
	C,0,2.760132,-1.714601,0.937854
	C,0,-3.359422,0.04301,1.139111
	C,0,-3.956891,0.581856,2.274001
	H,0,-4.242042,1.630664,2.31299
	C,0,-3.783457,-1.596342,3.295493
	B,0,-2.290494,-1.769414,-0.406833
	C,0,2.429167,-3.223874,3.323722
	H,0,2.313194,-3.794689,4.240078
	C,0,3.399614,-2.226354,3.232536
	C,0,3.561031,-1.483168,2.059458
	H,0,4.325604,-0.710929,2.015071
	C,0,-4.168249,-0.25833,3.367581
	H,0,-4.626398,0.132417,4.270887
	C,0,0.217203,4.872349,1.250867
	H,0,-0.827955,5.112035,1.430449
	H,0,3.938619,3.965841,0.754921
	H,0,3.304969,5.697248,2.378132
	O,0,-4.645036,0.211249,-2.39555
	C,0,-3.809228,-0.201931,-1.634408
	O,0,-3.360298,-1.411194,-1.493519
	O,0,3.025083,-2.052481,-1.581776
	C,0,2.186948,-3.033722,-1.700962
	O,0,2.219256,-3.971821,-2.455535
	H,0,7.501106,-0.054443,-0.510509
	H,0,0.910729,6.287859,2.717956
	H,0,-3.778347,6.468033,-1.102184
	H,0,-3.947501,-2.24645,4.150479
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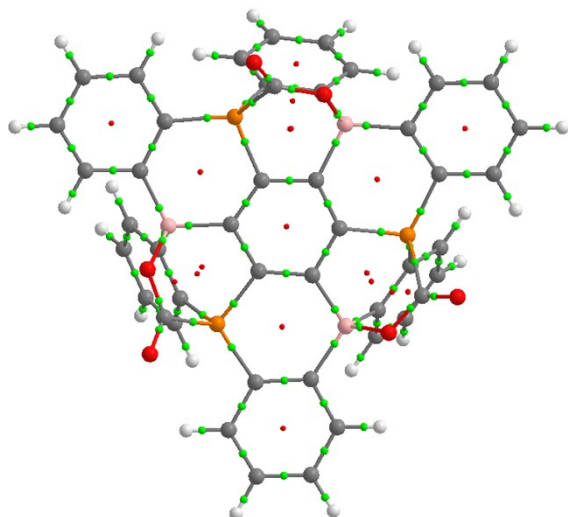
2CO₂-Al₃P₃-NG

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 C,-2.48910543,3.8242467075,-0.5144872821
 C,-1.2242940163,0.6103717569,-0.5792579253
 C,5.0798195747,2.6911418118,-1.2687070373
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 C,1.1250820601,1.0954934698,-0.7428286443
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 H,-2.3104152542,5.9752817419,-0.4893793178
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 C,-0.9619596336,-6.505828919,-0.6166118428
 H,-0.5977778414,-7.5247682357,-0.7041245328
 P,0.8077738324,-2.9025692986,-0.3996151126
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 C,-3.53808334,-1.0932408051,1.2003826122
 C,1.4554534643,-3.9298387675,2.134071032
 H,0.557881319,-4.5389648988,2.0566018555
 C,1.8254178069,-3.0610464859,1.1050214438
 C,0.3285536019,-1.1493875596,-0.5357672882
 C,-4.0475634118,-1.6302795079,2.3890286298
 H,-3.9748772332,-2.7020523903,2.5644516882
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 C,-3.6662002366,0.308982007,1.0534060938
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 C,-4.6512732376,-0.8322597516,3.3642000369

	<p>Al,-2.5701784671,-1.9728732104,-0.3146305366 C,2.2577886378,-4.0027967079,3.2716152452 H,1.9868920596,-4.6726568208,4.0823504263 C,3.4019930309,-3.2126876989,3.3615756222 C,3.7479814207,-2.3477277449,2.3200644212 H,4.6447987642,-1.7393708955,2.4235627591 C,-4.7589904775,0.5444767299,3.1804982619 H,-5.2250875906,1.1656935388,3.9394005547 C,0.8775858822,5.3063208891,1.3567428996 H,-0.066078179,5.8346990982,1.4883023903 H,4.2310231932,3.4176430299,1.0092047514 H,4.0073002142,5.2240020726,2.656151495 O,-4.5282243291,0.514481157,-2.666698003 C,-3.8482280411,-0.043685988,-1.8443459076 O,-3.6057979563,-1.3020401706,-1.7006393171 O,3.0810634729,-2.3740773794,-1.7462381536 C,2.0954175877,-3.2018939265,-1.8029938796 O,1.9023424066,-4.1084549911,-2.572619157 H,7.9278090213,0.8825101018,-0.8954480599 H,1.8672811358,6.4705326602,2.8821965668 H,-4.7016354498,6.4224039789,-0.8289563917 H,-5.0387728835,-1.2865985547,4.2721462268 H,-3.0414391355,-7.0627609527,-0.5893510847 H,4.0275568296,-3.2698188155,4.2485380587</p>
	<p>3CO₂-Al₃N₃-NG E= -3072,0995948H; FreqIm=0 C,-3.0008497043,-3.4787127001,3.3105373501 C,-2.7392470215,-2.061293964,0.9328050839 C,-1.9315462981,-3.1968242658,1.1271992912 C,-3.6171383841,-1.6046334742,1.9172214677 C,-3.7439615257,-2.3209317104,3.1056811822 N,2.3661016688,-1.6439238445,-0.3458189661 N,-2.6066511825,-1.2270531615,-0.3459619323 C,-0.1587732141,-1.4056561826,-0.3136133347 C,1.2384675477,-4.00674769,-0.5161211785 C,1.0776461513,-0.8174426999,-0.3152427296 C,-4.9706686914,-1.3325389438,-0.7732416181 H,-4.7998395266,-2.4065291833,-0.7950949312 C,-3.894914471,-0.4606553555,-0.5613443188 C,-1.2468148711,-0.5243283865,-0.3154207277 C,1.5125783654,-5.3807719004,-0.6912730989 H,0.6823593242,-6.0838880155,-0.6652389607 C,-4.0892156011,0.9307804367,-0.5170382804 C,2.3464127039,-3.1428508313,-0.5610286825 C,3.6392140427,-3.6387676896,-0.7733487038 H,4.4840694499,-2.9540559238,-0.7955472073 C,2.7891730188,-5.8819998548,-0.8986888536 Al,-0.5612759907,-3.2850546537,-0.2735705491 C,-6.2571398505,-0.8501850882,-0.9416080563 H,-7.073316039,-1.5464118638,-1.1077633287 C,-6.4886586809,0.5249470568,-0.8988895217 C,-5.4163411527,1.3801473059,-0.6920569195 H,-5.6103765398,2.4506678665,-0.6664290749 C,3.8644317555,-4.9940899772,-0.9418242987 H,4.8753442737,-5.3529498523,-1.1084056661 Al,-2.5644639486,2.1286422036,-0.274439341</p>

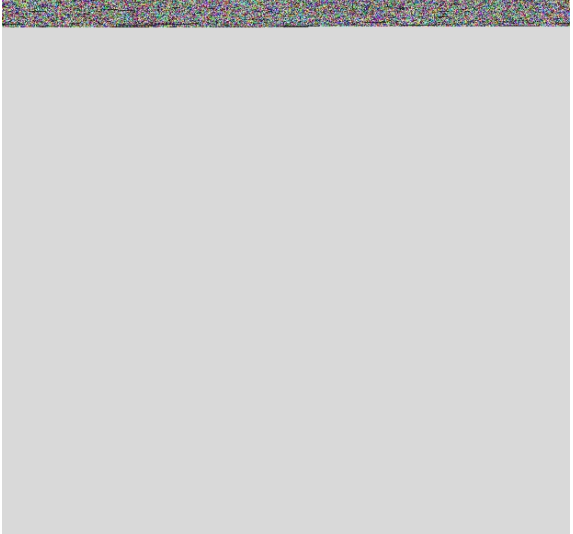
	<p> C,-1.1379934594,0.8405577224,-0.3138056656 C,3.6995882952,5.3567525882,-0.8977993539 C,1.5487601252,3.6036587263,-0.5603550815 C,2.8508644115,3.076044957,-0.5159033645 C,3.9037630054,4.0004959841,-0.6909087805 H,4.927788151,3.6330602459,-0.6651778201 C,1.3318998072,4.9713363195,-0.7720447478 H,0.3165257631,5.3607405007,-0.7939196349 C,2.3930528869,5.8440813817,-0.9403945329 H,2.198408631,6.8990482704,-1.1066342009 N,0.240722341,2.871294178,-0.3454743885 C,1.2968767056,0.565492088,-0.3134757571 C,3.7346982206,-0.0742489793,1.1270966523 C,0.4177247569,3.935032711,1.9179645191 H,1.4910228218,3.9938235074,1.781036001 C,-0.416078278,3.4031122631,0.9330223229 C,0.1692461816,1.3422281447,-0.3152551281 C,4.4212885405,0.1272919964,2.3308746121 H,4.8856843529,1.0934136658,2.5167177634 C,-1.8034369906,3.2710859246,1.1266400342 C,3.1551352557,-1.3415223057,0.9328298052 C,3.1989964401,-2.3302937738,1.9171010915 H,2.7134725682,-3.2892083727,1.7796963068 C,4.5138164398,-0.8594213393,3.3103076391 Al,3.1257516796,1.1565598203,-0.2736947257 C,-0.1399762148,4.4024816363,3.1063379451 H,0.5127916947,4.8164139435,3.8689223391 C,-1.5142773932,4.337319057,3.3104746263 C,-2.3219482599,3.7641743138,2.3303850446 H,-3.3908981901,3.6829097081,2.5156818562 C,3.8828593144,-2.0819585905,3.1054871427 H,3.9151483694,-2.8547988346,3.8674995016 C,-2.1001722609,-3.89206895,2.3310651526 H,-1.4955264081,-4.7771835748,2.5169747102 H,-4.2045729117,-0.7045209697,1.7799535963 H,-4.4292436247,-1.9622685483,3.8677310274 O,2.8188366296,-1.7440774734,-2.7417800362 C,3.0646673818,-1.0492676723,-1.8156732033 O,3.6837118805,0.0364148976,-1.6565321231 O,-1.8732340712,3.172213012,-1.6569940597 C,-0.6234889318,3.1792465167,-1.8158263271 O,0.101522427,3.3147588943,-2.7414541168 O,-1.8102199816,-3.2086541602,-1.6564184557 C,-2.4408812641,-2.1296935791,-1.8157056401 O,-2.9197903944,-1.5694633239,-2.7417817654 H,4.5430979879,6.0281534621,-1.0283929745 H,5.0546082554,-0.6694765214,4.233073987 H,2.9488410638,-6.9481946745,-1.0293878592 H,-3.1067581178,-4.0419053414,4.2333761347 H,-7.491944543,0.9196000863,-1.0293957941 H,-1.9496536983,4.7100338053,4.2332776308 </p>
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3CO₂-B₃P₃-NG

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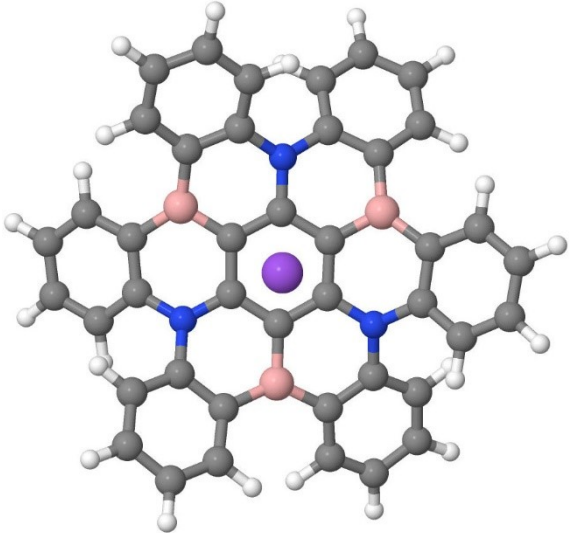
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 H,0,-0.303538,-5.686097,-0.758625
 C,0,-3.828754,1.190936,-0.587366
 C,0,2.232764,-3.465185,-0.551281
 C,0,3.322487,-4.343875,-0.643172
 H,0,4.338954,-3.956091,-0.643973
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 P,0,0.186367,3.099596,-0.455506
 C,0,1.299636,0.57969,-0.663914
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 C,0,-2.050977,2.671895,0.933881
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	<p>3CO₂-Al₃P₃-NG E= -3932,03045367H; FreqIm=0 C,1.817229,4.714914,3.25815 C,2.223534,3.10027,1.055707 C,0.98769,3.788079,1.149625 C,3.228456,3.20372,2.019486 C,3.018022,4.021457,3.129003 P,-2.976746,1.102693,-0.407477 P,2.443359,2.026837,-0.406728 C,-0.193508,1.420055,-0.397551 C,-2.199324,3.863605,-0.511105 C,-1.257472,0.526104,-0.40095 C,5.098874,2.344424,-0.731846 H,4.8186,3.39354,-0.790528 C,4.119038,1.354291,-0.558764 C,1.08436,0.826246,-0.401082 C,-2.615178,5.200634,-0.63033 H,-1.867819,5.991973,-0.606157 C,4.445735,-0.026668,-0.513493 C,-3.231869,2.890225,-0.558556 C,-4.579253,3.243857,-0.731413 H,-5.347652,2.476628,-0.79129 C,-3.951464,5.563833,-0.791816 Al,-0.283754,3.389382,-0.345008 C,6.437267,1.986052,-0.847878 H,7.191709,2.753982,-0.987554 C,6.794093,0.640937,-0.795696 C,5.811537,-0.334829,-0.634179 H,6.123204,-1.377727,-0.61128</p>

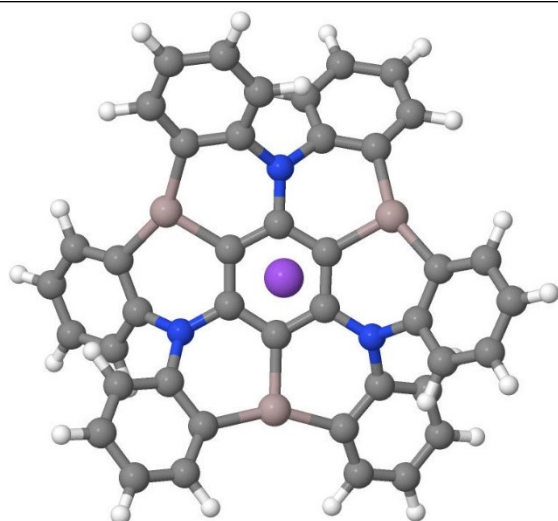
	C,-4.938023,4.582338,-0.845542 H,-5.980269,4.851914,-0.98518 Al,3.077427,-1.448642,-0.347325 C,1.326725,-0.542037,-0.398232 C,-2.842285,-6.204083,-0.791962 C,-0.886624,-4.243968,-0.557339 C,-2.24585,-3.836369,-0.512441 C,-3.195744,-4.865,-0.632414 H,-4.254714,-4.613236,-0.609938 C,-0.519291,-5.587966,-0.72825 H,0.529383,-5.869924,-0.786379 C,-1.499062,-6.567937,-0.842947 H,-1.211393,-7.605545,-0.980931 P,0.533799,-3.129025,-0.406537 C,-1.132809,-0.877507,-0.398011 C,-3.776642,-1.039292,1.145898 C,1.161979,-4.396431,2.019784 H,0.219484,-4.928886,1.916263 C,1.57423,-3.475071,1.055195 C,0.173426,-1.351743,-0.401042 C,-4.393146,-1.585451,2.278235 H,-4.406258,-2.665975,2.410016 C,2.788429,-2.749536,1.147158 C,-3.798121,0.374973,1.053535 C,-4.3918,1.192533,2.017105 H,-4.381934,2.274951,1.913421 C,-4.998929,-0.786679,3.251785 Al,-2.793128,-1.940302,-0.347576 C,1.977055,-4.623689,3.128041 H,1.67015,-5.336959,3.887128 C,3.178969,-3.931714,3.255044 C,3.569076,-3.009437,2.280214 H,4.511547,-2.480805,2.411935 C,-4.997849,0.600206,3.124363 H,-5.463995,1.222497,3.882391 C,0.82279,4.592264,2.284 H,-0.106741,5.142852,2.417529 H,4.161017,2.654427,1.914567 H,3.789825,4.112086,3.887457 O,-4.436153,0.779602,-2.67605 C,-3.829137,0.150284,-1.849412 O,-3.670716,-1.130688,-1.757749 O,2.81531,-2.614534,-1.756565 C,1.785474,-3.392662,-1.847599 O,1.544647,-4.234327,-2.673084 O,0.856345,3.746229,-1.754513 C,2.04492,3.243208,-1.847035 O,2.893482,3.45579,-2.673198 H,-3.614881,-6.962309,-0.884955 H,-5.472462,-1.24891,4.1138 H,-4.221909,6.612069,-0.884314 H,1.653184,5.353245,4.122209 H,7.837011,0.351145,-0.889633 H,3.815195,-4.10952,4.117965
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Table S5: Geometries, energies (in Hartree) and Cartesian coordinates (in Å) of the monomers with a Na⁺ cation in vacuum. Level of theory: M06-2X/6-311++G*//M06-2X/6-31+G*

	<p>B₃N₃-NG-Na down E=-2015,8763026H; FreqIm=0</p> <p>C,3.1964520981,-5.0122620729,1.4652648873 C,1.0563091798,-3.5345115334,0.4087354026 C,2.3625948499,-2.9967575471,0.3626171233 C,0.8270978721,-4.7764827284,1.0243825121 C,1.8891756855,-5.5048340954,1.5381515349 C,1.2263713355,-0.7418178439,-0.0695513405 C,3.7523048323,-0.7157233119,-0.5079103609 C,1.233341248,0.6787999617,-0.089844603 C,-1.0423065876,-4.7203823896,-1.2185485541 H,-0.0500780799,-5.1407774421,-1.3394576142 C,-1.2145986427,-3.4806831593,-0.5839746764 C,-0.0289318244,-1.4073464302,-0.0895169952 C,4.9221674872,-1.2995583117,-1.0349523292 H,5.017268742,-2.3817446644,-1.0174761968 C,-2.4958312423,-2.8915033196,-0.5086963206 C,3.6218836503,0.6883833104,-0.5842622241 C,4.609785945,1.4570060173,-1.21871335 H,4.4779206438,2.526408079,-1.3404309106 C,5.9196225555,-0.5393115021,-1.6211187286 B,2.521752492,-1.5288430049,-0.0744587613 C,-2.140170477,-5.3988277243,-1.7246266123 H,-1.9882509669,-6.3499871075,-2.2257758453 C,-3.4256222166,-4.8562100914,-1.6235907839 C,-3.5858097332,-3.6124330424,-1.0372920029 H,-4.570427043,-3.1534047476,-1.0211424745 C,5.7467381431,0.845118029,-1.7234568633 H,6.4948197954,1.4519362264,-2.2245151119 B,-2.5849701867,-1.4194608221,-0.0745625653 C,-1.2557624123,-0.6910373398,-0.0692587182 C,-2.4937099631,5.3954074796,-1.6212496026 C,-2.4073414836,2.792511545,-0.5824209368 C,-1.2564791445,3.6075146472,-0.5075620316 C,-1.3361580178,4.9120744757,-1.0357288594 H,-0.4463566666,5.5353314498,-1.0197831747 C,-3.5675100874,3.2633800082,-1.2160676121 H,-4.4278486685,2.6144395187,-1.3366151601 C,-3.606466874,4.5535132603,-1.7217011043 H,-4.5065251778,4.8976836304,-2.220855984 C,0.0293169113,1.4331404853,-0.069306993 C,1.4141495108,3.544653965,0.3620471809 C,-4.550653376,1.6714241136,1.0250606552 H,-4.3831842686,2.7387722486,1.1167673064 C,-3.5892314085,0.8522819387,0.40961906 C,-1.2044435158,0.7288200956,-0.0889808843 C,1.5566688752,4.8412042282,0.8965971461 H,0.6938781178,5.5017705829,0.8936430009 C,-3.7768116084,-0.5478191216,0.3623861437 C,2.5330686194,2.6823111593,0.4077660581 C,3.7236474452,3.1050159146,1.0224214385 H,4.564483456,2.4263983879,1.1129592071 C,2.743286582,5.2749233026,1.4633330686</p>
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	<p>B,0.0631733669,2.9484817886,-0.074418341 C,-5.713050363,1.1155883797,1.5373953537 H,-6.4413558249,1.763106513,2.0163180508 C,-5.9402611969,-0.2627201112,1.4631969022 C,-4.9712068917,-1.0730406831,0.8959956513 H,-5.1120777041,-2.1504824853,0.8916856078 C,3.8236159575,4.3891368352,1.5357904326 H,4.7488731275,4.695758962,2.0143079058 C,3.4141203866,-3.7681058506,0.897807611 H,4.4175043193,-3.3510114342,0.8946426938 H,-0.1809994871,-5.1650373522,1.1159376614 H,1.6921333096,-6.4590116411,2.0175336795 H,-2.5286611053,6.4002568471,-2.0293774985 H,-6.8504037128,-0.6910544737,1.870412121 H,2.8275126421,6.2768840688,1.8715131003 H,4.0220356457,-5.5859895536,1.873759171 H,6.8076200725,-1.0118360847,-2.0282360647 H,-4.2784126957,-5.3887499391,-2.0318534055 N,2.4482113151,1.3436270345,-0.0899086808 N,-0.0606242549,-2.7918455629,-0.0890989813 N,-2.3875626576,1.4485763512,-0.0878646406 Na,0.000354351,-0.000134316,2.2071298451</p>
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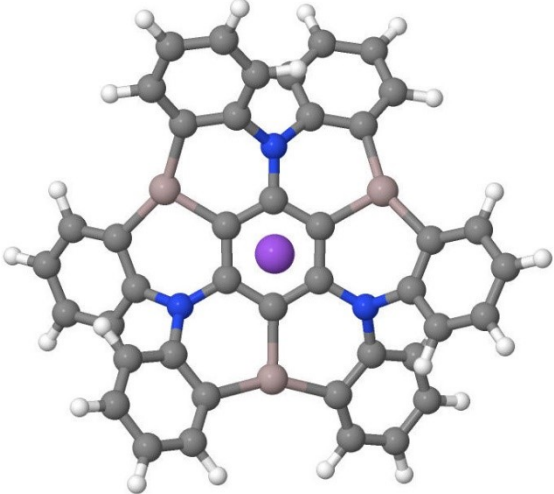
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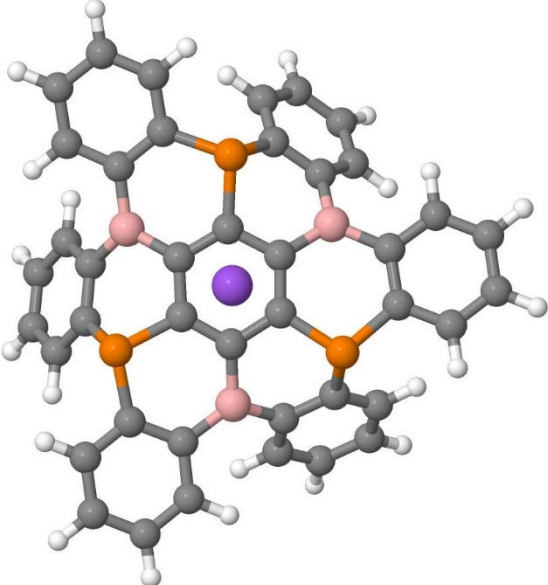


Al₃N₃-NG-Na down

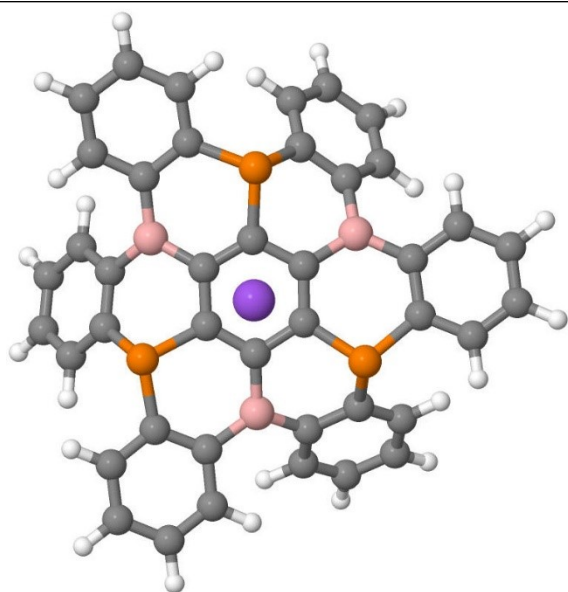
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 C,1.2132473892,-5.5874620846,2.0348132997
 C,1.2185774708,-0.7452143767,-0.0453308149
 C,4.1179224585,-0.4722836087,-0.7710518391
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 C,-0.0370745075,-1.4047271859,-0.0645688484
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 H,5.6876419114,-1.7822049917,-1.4601183278
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 C,-3.317329236,-4.221349424,-1.4551362666
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	<p>H,-3.0488344407,5.1607873531,-0.6832426841 C,-4.43747026,1.5681733613,-0.8913128894 H,-4.839039535,0.5601542682,-0.9473238371 C,-5.0860385116,2.6059628491,-1.5468303003 H,-5.9779478733,2.3939038942,-2.1289967993 N,-2.7469234697,0.6557234214,0.5689948823 C,-0.406516017,1.3689740346,0.5363137175 C,0.6017626708,4.1008390791,1.2618880451 C,-4.6958172255,0.6380953823,1.9898605188 H,-4.6060742494,1.7199565318,2.0177430525 C,-3.7486146922,-0.1160900336,1.2762089434 C,-1.3665069424,0.3250014456,0.5560118612 C,0.630648075,5.3319390521,1.9464492603 H,-0.2614544341,5.95449718,1.9500714172 C,-3.8518843481,-1.5291274932,1.2635727747 C,1.7740148246,3.3051544912,1.2747851427 C,2.9006925104,3.749038479,1.9881826436 H,3.7929488052,3.1307216414,2.0163013881 C,1.7572218979,5.7808385104,2.6205936873 Al,-0.9573304723,3.1842185368,0.6317176778 C,-5.7479748815,0.0215583492,2.6510110329 H,-6.4609717475,0.6305088798,3.1987704886 C,-5.8841090695,-1.3676044486,2.6228421275 C,-4.9324624512,-2.1192100492,1.9485752451 H,-5.0259276473,-3.2030448716,1.9523096068 C,2.8924603772,4.9687156895,2.648948111 H,3.7762347715,5.2821873069,3.1965878235 C,4.3009243724,-3.212345246,1.9501287334 H,5.286193562,-2.7511818755,1.9548075299 H,0.8131380401,-4.8498281762,2.01621291 H,2.6833709202,-5.9116932354,3.1980498306 H,-5.1071702802,4.7254086311,-1.9616803912 H,1.7507733004,6.7381434045,3.1319183201 H,6.6471546244,2.0576215728,-1.9605639845 H,4.9572057066,-4.8859580798,3.1358291266 H,-1.5402147521,-6.7844605596,-1.9626912084 H,-6.7100539259,-1.8514987312,3.134297582 Na,0.000542519,-0.00029574,-1.6969531605</p>
	<p>B₃P₃-NG-Na down E=-2875,58769211H; FreqIm=0 C,4.8390229395,1.0124233562,2.4484298896 C,3.7072449732,-0.3499629495,0.2849725533 C,3.3957429885,1.0215638823,0.4718635609 C,4.5944309388,-1.0055822553,1.1382700167 C,5.1551460079,-0.3247694179,2.2202655671 P,-0.4831850514,3.1688789835,-1.2008282056 P,2.985768336,-1.1665660178,-1.2012720412 C,1.146874283,0.8598835464,-0.9351833253 C,2.2976530359,3.2961808251,-0.5817969505 C,-0.1482617312,1.3957439471,-0.9776836848 C,4.1061982025,-3.6631165695,-1.0406043844 H,5.0214691416,-3.1337652575,-1.2989118398 C,2.912166701,-2.9529467273,-0.8627177066 C,1.2827606501,-0.5694286432,-0.9776977529 C,3.4890964467,4.045517648,-0.503183862 H,4.4283043289,3.5254596639,-0.3332528931</p>

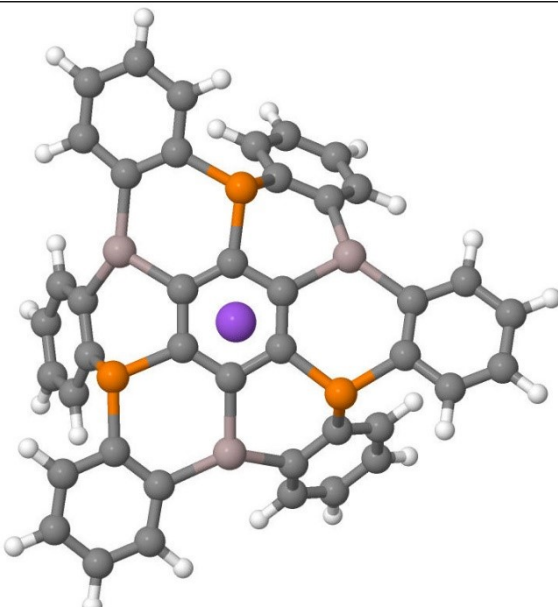
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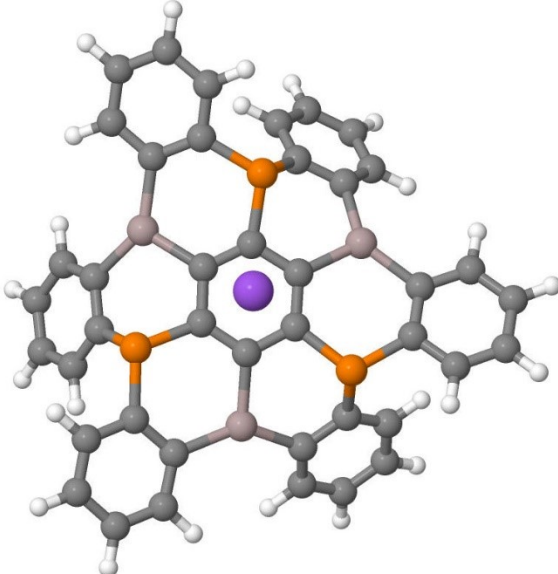


B₃P₃-NG Na up

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 C,-1.398623256,0.0963483012,0.2981966615
 C,3.7977611315,-3.976000091,0.544045782
 H,3.2891519921,-4.9055155827,0.7925698348
 C,3.0570294027,-2.8070536639,0.3248056855
 C,0.6155456017,-1.2591250362,0.2990896095
 C,-3.9376403305,-3.6411195342,0.0417225873
 H,-3.3932930595,-4.5693178219,-0.1076101357
 C,3.7118442502,-1.5779830776,0.0600408278
 C,-3.9596671867,-1.2446199535,0.3227796089
 C,-5.3422695278,-1.3023346382,0.5425112334
 H,-5.893010437,-0.3977078602,0.7930583185
 C,-5.3121817978,-3.6930960903,0.2401838522
 B,-1.6791810217,-2.4250741253,-0.1500359546
 C,5.1873733305,-3.957445308,0.4779987268
 H,5.7481936237,-4.8736436669,0.6368069772
 C,5.85383947,-2.7544553007,0.2467448287
 C,5.1220602582,-1.5897088482,0.048450772
 H,5.6541464125,-0.6541111298,-0.0989504574
 C,-6.0208429678,-2.5150413385,0.4742382134
 H,-7.0946073588,-2.5431721316,0.633590312
 B,2.9401688189,-0.2413441943,-0.1460629527
 C,1.429964752,-0.1169397649,0.2717507407
 C,-0.5422793685,6.4471687968,0.2401665072
 C,0.9014683274,4.0513840144,0.3224458553
 C,-0.4899947396,4.0037085899,0.0557880303
 C,-1.1848363259,5.2308972799,0.0420762531
 H,-2.2609269434,5.2238339337,-0.1066964813
 C,1.5431329833,5.2775386297,0.541635197
 H,2.6020547791,5.3019995463,0.7917096113
 C,0.8324163143,6.4716774349,0.4734724089
 H,1.3452250911,7.4155742015,0.6323392902
 P,1.8893432694,2.5597190649,0.637526094
 C,-0.6140075003,1.2972938203,0.2698665564
 C,-2.6163132101,2.581764598,-0.9334636078
 C,3.5723061472,3.3566884215,-1.4951611158
 H,3.2110334702,4.3685220189,-1.335997828
 C,3.084038681,2.2991016585,-0.7311117002
 C,0.782282879,1.1630117102,0.2990936635
 C,-2.8969087614,3.4825887272,-1.9771929229
 H,-2.1874756143,4.2749093201,-2.1993323293
 C,3.5445937819,0.973958355,-0.9300168997
 C,-3.5337768074,1.5208234817,-0.7325806393
 C,-4.6945448891,1.4143602424,-1.4954184802
 H,-5.3904144946,0.5961159545,-1.3345140013
 C,-4.043053907,3.367279281,-2.7596239573

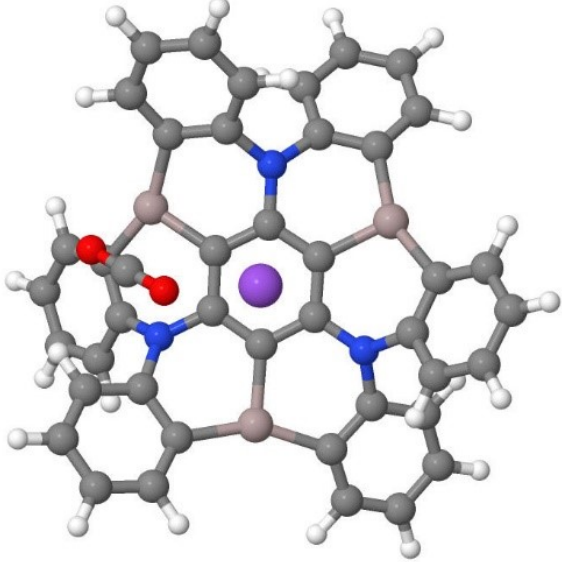
	<p>B,-1.261421534,2.6668149254,-0.1497716779 C,4.4987928048,3.1118521323,-2.509303056 H,4.8584756697,3.9367397785,-3.1172721036 C,4.9392363004,1.8146709313,-2.7563137869 C,4.4657329298,0.7653390616,-1.9728016006 H,4.7975827739,-0.2454266513,-2.1933597914 C,-4.946391765,2.3379112443,-2.5104799245 H,-5.8411589945,2.2365212078,-3.117541394 C,-1.5680815759,-4.2482439848,-1.9781743652 H,-2.6091211158,-4.0300773186,-2.1997511746 H,2.178782051,-4.9640721199,-1.3367577074 H,0.9834457664,-6.17324788,-3.1208474666 H,-1.1104245219,7.3720855982,0.2253556976 H,-4.2272550768,4.0741103019,-3.5625768125 H,-5.828981023,-4.6476499453,0.225134731 H,-1.4151945879,-5.6946452436,-3.564850357 H,6.9389355617,-2.7248777952,0.233559116 H,5.6441060663,1.619892579,-3.558487237 Na,-0.0007121682,0.0006620279,2.5836951722</p>
	<p>Al₃P₃-NG-Na down E=-3528,24683866H; FreqIm=0 C,4.8756273843,0.5762851361,2.7494393179 C,3.7120220458,-0.4625282468,0.4149977653 C,3.7331490936,0.9434733133,0.6201983581 C,4.2681298721,-1.3186934082,1.3694852493 C,4.8467226756,-0.7970720924,2.5310813209 P,-0.6001062386,3.2026268269,-1.2310258405 P,3.0735091276,-1.0814428175,-1.2302134476 C,1.1346375157,0.8731406961,-1.1007585769 C,2.2196273635,3.8994301614,-0.7288079514 C,-0.1655416582,1.3944418147,-1.1016644882 C,4.5664106971,-3.3305191249,-1.3308391842 H,5.319057315,-2.6006714732,-1.6240798022 C,3.2508143767,-2.9138767594,-1.0742014467 C,1.2902145074,-0.5540031088,-1.1014059664 C,3.1891674435,4.9137948177,-0.6271736417 H,4.2145238942,4.6532874365,-0.3699500188 C,2.267496265,-3.8719262175,-0.7274307482 C,0.8983086463,4.2720873136,-1.0756045715 C,0.6016115225,5.6196299096,-1.332862172 H,-0.4067368555,5.9065225357,-1.6261930677 C,2.8801036509,6.2522027823,-0.852959899 Al,2.6108964083,2.0225538108,-0.5497402468 C,4.9293991583,-4.6691870532,-1.2088118106 H,5.9546899899,-4.9687867985,-1.4043357748 C,3.9752794753,-5.6199612897,-0.8504187865 C,2.6614319837,-5.2186487239,-0.6253851532 H,1.9233198246,-5.9764390065,-0.3678773328 C,1.5797303523,6.6031747196,-1.2114360578 H,1.3268390887,7.6408622885,-1.4074799579 Al,0.4463303179,-3.2724629005,-0.548785738 C,0.188761407,-1.4194496379,-1.1003296458 C,-6.8545676446,-0.6325453486,-0.8491306285 C,-4.1488627162,-1.3582198776,-1.072412381 C,-4.4868778548,-0.0272782082,-0.7268234802 C,-5.8501833389,0.3049303373,-0.6250609824</p>

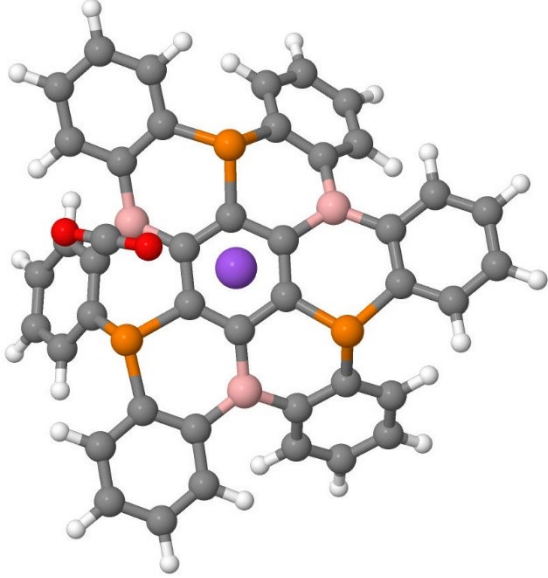
	<p>H,-6.1375103001,1.3232288793,-0.3683913529 C,-5.1673781304,-2.2895462922,-1.3280556259 H,-4.9115006658,-3.306476739,-1.6204845624 C,-6.5081875536,-1.9345384485,-1.2062712489 H,-7.2802723069,-2.6728884297,-1.4009546812 P,-2.4734820084,-2.1210325584,-1.2285779845 C,-1.3237370694,0.5461213479,-1.1004044835 C,-2.6829308684,2.7621717156,0.6201579184 C,-3.2759391449,-3.0375810246,1.3709724984 H,-4.2062780999,-2.4971077923,1.2181972961 C,-2.2563033508,-2.9832342638,0.416561633 C,-1.1249598281,-0.8405167942,-1.1007646001 C,-3.3955203926,3.0180479877,1.801582036 H,-4.3360254598,2.5014293701,1.987483256 C,-1.0491113896,-3.7043895994,0.6215180107 C,-1.4549681782,3.4470608502,0.4141887363 C,-0.9920238636,4.3579971414,1.3678222503 H,-0.0589668454,4.8935982948,1.2142869355 C,-2.9362043574,3.9363741061,2.7487486796 Al,-3.0570891385,1.2502543448,-0.5490345954 C,-3.1132964973,-3.7997530108,2.5323440694 H,-3.9157720115,-3.8359291866,3.2636808552 C,-1.9381181964,-4.5110051395,2.7506181242 C,-0.9137600353,-4.4497371783,1.8027197756 H,0.0039893254,-5.0060121919,1.9879323571 C,-1.7330240997,4.5987634656,2.5294159032 H,-1.3630498514,5.3124648161,3.2600872899 C,4.3109844263,1.4330644512,1.8015042853 H,4.3341596869,2.5059743962,1.9868425467 H,4.2647568465,-2.394618614,1.2167527546 H,5.2787475993,-1.4742318905,3.2624702546 H,-7.8988141486,-0.3485352767,-0.7606187482 H,-1.8197489737,-5.119111589,3.6473074999 H,-3.5154356989,4.1346365247,3.6455848255 H,5.3366678483,0.9790388801,3.6463097842 H,3.6483638293,7.0144135371,-0.7647610449 H,4.2514827164,-6.6662870647,-0.7615841965 Na,-0.0006829098,-0.0001342617,1.1905793367</p>
	<p>Al₃P₃-NG-Na up E=-3527.61892303H; FreqIm=0 C,-5.1175224142,2.0798414439,-2.8599208739 C,-3.9114683475,0.6460030319,-0.7705121071 C,-3.5425736371,1.9974864103,-0.9936845543 C,-4.8630595667,0.0352337534,-1.5902345451 C,-5.4606954552,0.7523251319,-2.6297688971 P,1.4264215105,2.9125680305,0.74011197 P,-3.2349710548,-0.2206985269,0.7362983174 C,-0.8533881748,1.1506054913,0.4592628734 C,-1.0751796369,4.3483950944,0.1676063991 C,0.5420825793,1.2972412547,0.4514824624 C,-5.2519659996,-2.0078141637,0.9693134033 H,-5.7649446757,-1.1149596986,1.3232644662 C,-3.9014051461,-1.9357148885,0.5916025713 C,-1.3931295542,-0.1798341831,0.4519141204 C,-1.7478461016,5.5830799537,0.1087463049 H,-2.7883685608,5.6122754295,-0.2105387721</p>

<p> C,-3.2281106242,-3.1053584278,0.1661883203 C,0.2725085726,4.3464451829,0.5992120658 C,0.8821045439,5.5510542281,0.9849657071 H,1.9102049045,5.5485337643,1.3435823708 C,-1.1252393301,6.7792126683,0.4541660955 Al,-1.9640445923,2.6575042174,-0.0881763954 C,-5.9554777149,-3.2057641533,0.8825181692 H,-7.0031964071,-3.2367168456,1.1665022237 C,-5.3112684986,-4.3613236877,0.4432225566 C,-3.9620467899,-4.3046251464,0.1056616396 H,-3.4663130559,-5.2216192729,-0.2087371349 C,0.195362144,6.7589618681,0.8999804095 H,0.6899399421,7.6811623739,1.1902075681 Al,-1.318353147,-3.031669776,-0.0833926038 C,-0.5683959713,-1.3150796973,0.4595566 C,6.4354632032,-2.4124569573,0.4368355547 C,3.6301867245,-2.4071097965,0.5899625698 C,4.3041219942,-1.2411601256,0.1552860443 C,5.7096013287,-1.275729354,0.0924617418 H,6.2541232773,-0.3893549981,-0.2289760112 C,4.3700831377,-3.536910284,0.9743713477 H,3.8551246654,-4.4257401812,1.3354780449 C,5.7592083514,-3.5458858399,0.8854215547 H,6.3116367084,-4.4348592838,1.1749684039 P,1.812312213,-2.689485907,0.739467612 C,1.4245219948,0.1646758206,0.4563459528 C,3.4992257997,2.0747731776,-0.9959725573 C,2.4025774919,-4.243877922,-1.5763696582 H,3.4425956674,-3.9719696907,-1.4242847097 C,1.3983866456,-3.7181318062,-0.7603394419 C,0.8537483641,-1.1172521304,0.4506051923 C,4.3997259894,2.265679353,-2.0546802502 H,5.1563040652,1.5108220944,-2.263098049 C,0.0431114855,-4.0743746057,-0.9811446864 C,2.514778478,3.0701307986,-0.7663143552 C,2.4619996087,4.2041011643,-1.5798071294 H,1.7078250686,4.9686649004,-1.4207490775 C,4.3564903681,3.4064346074,-2.8569099365 Al,3.2833087714,0.3743022085,-0.0959047279 C,2.0794022868,-5.1265566184,-2.6100099972 H,2.8715123479,-5.5232663787,-3.2384831067 C,0.75773513,-5.4929862786,-2.8379000832 C,-0.2475323779,-4.9554371989,-2.0334217801 H,-1.2806335507,-5.2342334624,-2.2350327576 C,3.380162494,4.3674918937,-2.6200506208 H,3.3229659901,5.2529390984,-3.2465320806 C,-4.1548230352,2.685523479,-2.0518359552 H,-3.8796026285,3.7192328841,-2.255218035 H,-5.1472371432,-1.0012445108,-1.4363651072 H,-6.1958765497,0.2617077461,-3.2611003612 H,7.5193060303,-2.4115358718,0.3715608099 H,5.073595909,3.5388596021,-3.6613024651 H,-1.6676896069,7.7177387152,0.3916846213 H,-5.5887336716,2.637296439,-3.6636688513 H,-5.8534400421,-5.2999407802,0.3797275742 H,0.5097549115,-6.1847194136,-3.637164763 Na,0.0044313633,0.0002165528,2.7141327995 </p>

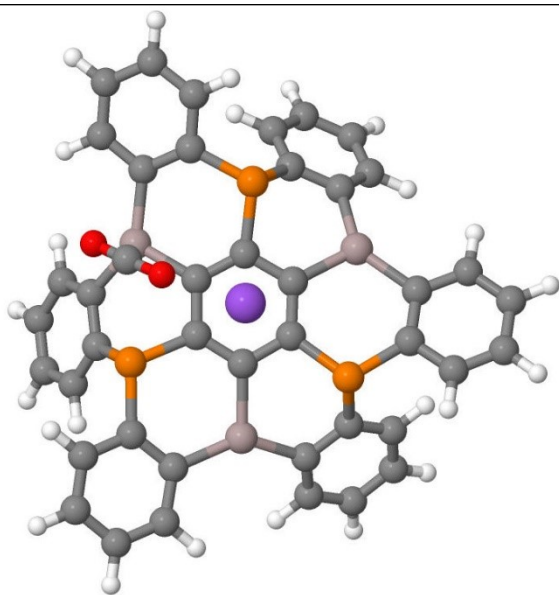
Table S6: Geometries, energies (in Hartree) and Cartesian coordinates (in Å) of the complexes with a Na⁺ cation in vacuum. Level of theory: M06-2X/6-311++G*//M06-2X/6-31+G*

	<p>B₃N₃-NG-Na:CO₂ E=-2203.88563344H; FreqIm=0</p> <p>C,2.7722643182,-5.4696401673,1.6329572485 C,0.7935310295,-3.6646217664,0.8054111949 C,2.1533258328,-3.3442963893,0.5994852044 C,0.4375626107,-4.8523291512,1.4623680882 C,1.4200551273,-5.744410349,1.863166072 C,1.3447646263,-0.9341542936,0.2610794382 C,3.7839180776,-1.3016130506,-0.4304372726 C,1.5808046013,0.465809086,0.2568977265 C,-1.6086500849,-4.500418396,-0.5963724595 H,-0.7141351196,-5.0878510446,-0.7704140341 C,-1.523189168,-3.2451890386,0.0299968953 C,0.0082333349,-1.3875153692,0.4183032114 C,4.7875634618,-2.0565383514,-1.0709713079 H,4.708498284,-3.1401685951,-1.0597691604 C,-2.6833586442,-2.4520879874,0.1851312822 C,3.8770040271,0.1077600965,-0.4867852912 C,4.9150824977,0.7161122789,-1.2127292275 H,4.9561697986,1.7950698692,-1.3110277072 C,5.836192785,-1.4583063175,-1.7487505008 B,2.4928151287,-1.9161675414,0.1400337875 C,-2.8367828385,-4.9858175149,-1.0183962774 H,-2.8811562299,-5.9538402342,-1.5083842822 C,-4.0038036286,-4.2341603607,-0.8420501169 C,-3.9121393924,-2.9808051531,-0.2611572657 H,-4.8044163226,-2.3663375025,-0.1731645209 C,5.8834873225,-0.0623516499,-1.8276614059 H,6.6734495693,0.4253019696,-2.3908990326 B,-2.501064207,-0.9935598778,0.6389538939 C,-1.0803826834,-0.4841566196,0.5261741483 C,-1.5139987146,5.6933416813,-1.0592733165 C,-1.7262744197,3.1281165799,0.0701480144 C,-0.4568670889,3.7411618853,-0.0353012595 C,-0.3877844607,5.0291944297,-0.6030062099 H,0.5879709297,5.4941611996,-0.714968501 C,-2.8668920379,3.788216866,-0.4214000818 H,-3.8413737511,3.31465845,-0.3768552368 C,-2.7556355764,5.0559055602,-0.9736763813 H,-3.6477966647,5.5450547905,-1.3532040209 C,0.5162307663,1.4031729783,0.3476097118 C,2.246587128,3.2812285106,0.5710206687 C,-3.840648175,2.3446305677,1.919036252 H,-3.481888884,3.3630199582,2.0208251331 C,-3.0893966958,1.3970419135,1.208283775 C,-0.8026927518,0.9073818276,0.507374666 C,2.6372026386,4.5503464457,1.0439356491 H,1.8929260886,5.3405764158,1.0908473961 C,-3.5077070294,0.0491962057,1.1556235126 C,3.2130788171,2.2517230224,0.5643216219 C,4.5004470998,2.486900687,1.0704860779 H,5.2210162539,1.6787370489,1.1309712098 C,3.9203512948,4.7978934709,1.5010664689 B,0.785233229,2.8924627477,0.2936196473 C,-5.032501522,1.9729867295,2.5220113567 H,-5.5957745537,2.7141796058,3.0808522051 C,-5.4937049051,0.6545635636,2.4422651094 C,-4.7252882061,-0.2881967519,1.7809154927 H,-5.0402838085,-1.328013124,1.7809326063</p>
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	<p>C,4.8464540443,3.7496877784,1.5261416437 H,5.8419993532,3.9119569708,1.9280086202 C,3.1217625836,-4.2762137604,1.0242713494 H,4.1723995908,-4.0251591827,0.9076245434 H,-0.6026186482,-5.065408605,1.6829541156 H,1.1293891212,-6.6521282684,2.3832531029 O,-2.0870494673,0.7326439218,-2.4580865442 C,-3.2030380707,0.9731823455,-2.1896972327 O,-4.3057432827,1.2047047128,-1.9476717228 H,6.5950551334,-2.0611360601,-2.2369600684 H,-1.4339525307,6.6831815586,-1.4967221559 H,-6.4228752578,0.3697015266,2.9249769618 H,-4.9604523651,-4.618952859,-1.1803259397 H,3.5361405831,-6.167798598,1.9594618654 H,4.1959415345,5.7808488113,1.8690684134 Na,0.0183475764,0.0088326872,-1.9243507355 N,2.8766810858,0.9339782374,0.1156811839 N,-1.8596345991,1.8037710783,0.5952963971 N,-0.2408956694,-2.7512823495,0.4227328166</p>
	<p>Al₃N₃-NG-Na:CO₂ E=-2856.41359738H; FreqIm=0 C,1.9669638272,-5.8751688115,2.1294904345 C,0.5381426521,-3.7545551363,0.9384124667 C,1.9518490171,-3.7916459736,0.8391030255 C,-0.1256696847,-4.7615781484,1.661609978 C,0.5774722265,-5.80499918,2.2451678627 C,1.304445968,-0.9305240218,0.204331511 C,4.1754168631,-1.1494074118,-0.5742049491 C,1.5561878211,0.4654112822,0.2080034328 C,-1.3237837475,-4.4255816266,-1.1114382216 H,-0.3127724805,-4.7791968807,-1.2950193639 C,-1.5212147791,-3.317616817,-0.2718143084 C,-0.0383151302,-1.3743471882,0.2976913155 C,5.2567549018,-1.6548779299,-1.3218746057 H,5.4733024368,-2.7202596305,-1.2819767499 C,-2.8354267964,-2.8515447646,-0.0209179802 C,3.916371587,0.2426131713,-0.6414186564 C,4.712663781,1.0562466178,-1.466684267 H,4.5098296959,2.1222551159,-1.5194031026 C,6.0604569282,-0.8418983301,-2.1104906179 Al,2.7419980191,-2.1694625031,0.2003970969 C,-2.4028405971,-5.0912955499,-1.6782845518 H,-2.2237649939,-5.9472424188,-2.32219874 C,-3.7062149034,-4.6635438942,-1.4217034181 C,-3.9039868547,-3.5498819054,-0.6140473891 H,-4.9215907632,-3.2084644079,-0.4368785983 C,5.7701595447,0.5212142949,-2.1896088417 H,6.3696245187,1.1734112029,-2.8178311807 Al,-2.8865588087,-1.0736155983,0.7175277275 C,-1.1175312867,-0.4591537871,0.3532632425 C,-2.2994606294,5.5705821071,-1.5346739286 C,-1.9421853956,3.107841925,-0.2153919396 C,-0.853673294,4.0099426059,-0.3159677622 C,-1.0705549037,5.2305807134,-0.9853259539 H,-0.2484828856,5.9377725019,-1.0726987262 C,-3.1835569342,3.4535676158,-0.7804394618 H,-4.0248330865,2.7733200535,-0.672399454 C,-3.3589372539,4.6670048882,-1.4309416141 H,-4.3284106699,4.9085553106,-1.8567637269 C,0.5001747337,1.4071785548,0.2573503352 C,2.6860657749,3.3980092595,0.7230461593 C,-3.3430479638,2.7612355201,2.1912060088 H,-2.7882781721,3.6874966878,2.0746107173</p>

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	<p>B₃P₃-NG-Na:CO₂ E=-3063.54419899H; FreqIm=0 C,2.8452886594,-4.6608265484,2.1571975473 C,0.9643326655,-3.7316303177,0.3196564867 C,2.213064439,-3.0683544064,0.4103106077 C,0.6844009586,-4.8551342605,1.0944656881 C,1.6259688408,-5.317192906,2.014593207 C,1.2826207789,-0.8174179772,-0.6731082882 C,3.958883664,-1.2862440633,-0.730450212 C,1.4518187083,0.5751411847,-0.7027504591 C,-2.3021172891,-4.8588666538,-0.6621400392 H,-1.5726189158,-5.5876943563,-1.0100954816 C,-1.9172676116,-3.5285444928,-0.4465414678 C,-0.0564791168,-1.3224506673,-0.5751988737 C,5.0017351992,-2.230526996,-0.8304493376 H,4.7764534366,-3.281037976,-0.6696481703 C,-2.8716569121,-2.5585110093,-0.049889318 C,4.2805704733,0.0645631089,-1.0161912358 C,5.5885457133,0.4274477567,-1.363834727 H,5.8166640522,1.458264819,-1.627953442 C,6.302550581,-1.8648215606,-1.1551348195 B,2.5130467571,-1.751925251,-0.3863873879 C,-3.6205765059,-5.2560945141,-0.4643178988 H,-3.9020825441,-6.2930220787,-0.6216224376 C,-4.5822542942,-4.3120409445,-0.1035770499 C,-4.2075833687,-2.9881895562,0.0909035716 H,-4.9713466604,-2.2552287329,0.3361191937 C,6.6010542028,-0.5257923139,-1.4060588355 H,7.6130747095,-0.2283735128,-1.663950874</p>

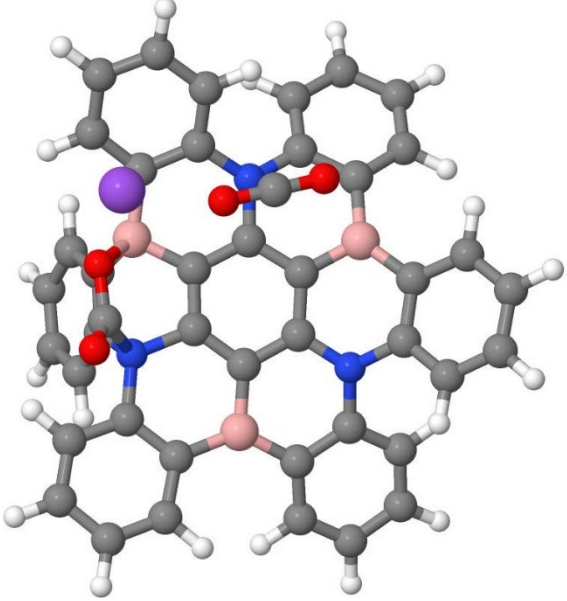
	<p> B,-2.5107105461,-1.0571799522,0.1524646224 C,-1.164440106,-0.4782847106,-0.4155800514 C,-1.2576033556,6.3719538416,-0.3271312508 C,-1.9174116964,3.6538229585,-0.3487770584 C,-0.5550714561,4.0259014427,-0.2291574373 C,-0.2625025015,5.4053089908,-0.2419072927 H,0.7758451612,5.7226198993,-0.2046505376 C,-2.9173255526,4.629488633,-0.4529269947 H,-3.9559359496,4.3337170602,-0.5883018468 C,-2.593702379,5.9821304103,-0.4146737963 H,-3.3795815708,6.7282938483,-0.4835403427 C,0.3514622117,1.4842836359,-0.5580993018 C,1.9898357711,3.3060002012,0.4945552388 C,-4.0287269486,2.1659908694,1.7218731565 H,-4.0038919461,3.2416294891,1.5724036228 C,-3.3372924361,1.313420905,0.8644240207 C,-0.934458658,0.9354273877,-0.4557797841 C,2.0922298396,4.2458201805,1.5365392272 H,1.2045069756,4.7867414011,1.8523309832 C,-3.3589436344,-0.0912313986,1.048634286 C,3.1577466597,2.5716975061,0.1709521506 C,4.3680808607,2.8170971483,0.8156971046 H,5.2569936607,2.2470836731,0.5617147904 C,3.293222544,4.47840839,2.2018164337 B,0.5987641682,2.9818213571,-0.1514922776 C,-4.723024662,1.6408650971,2.8124739304 H,-5.2409980146,2.3116675923,3.4915737533 C,-4.7310979924,0.2678259151,3.0416944144 C,-4.0581535683,-0.5810528773,2.1664050724 H,-4.0516987477,-1.6483654194,2.3702693097 C,4.4332629928,3.7701058388,1.8327357104 H,5.3740342427,3.9409388435,2.3476923584 C,3.1291715837,-3.5540160234,1.3611843016 H,4.0739605791,-3.0359007022,1.5004871655 H,-0.2765491571,-5.3557016921,1.0177476575 H,1.3933482211,-6.17933904,2.6326951134 O,-2.1318662591,-0.2537554135,-3.5303601335 C,-3.1614008733,-0.3852383689,-2.9824827471 O,-4.1767736462,-0.5335139052,-2.4570066205 H,7.0792916735,-2.6199784926,-1.2252702009 H,-0.9943128036,7.4251040987,-0.3368126769 H,-5.2548963302,-0.1399954144,3.9005312071 H,-5.6206308453,-4.6070067825,0.0117520036 H,3.5701405641,-5.0061801297,2.8876601226 H,3.3375243266,5.204939015,3.0070892957 Na,0.0581318767,0.0832283555,-2.9203259341 P,3.0138840357,1.354387484,-1.1943034654 P,-2.4401282958,1.9347017263,-0.6108059809 P,-0.2203088068,-3.0934088565,-0.9288507583 </p>
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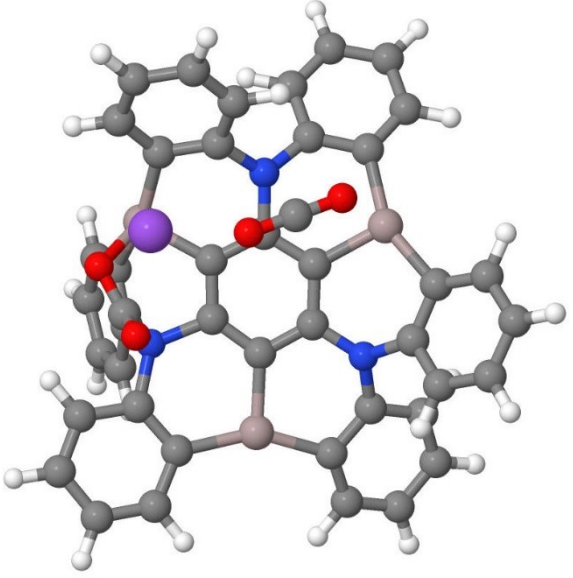


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 C,1.4547401584,0.5575879378,-0.7586971369
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 H,-1.2903052244,-5.6250056744,-1.5038137501
 C,-1.9422678812,-3.759478061,-0.6224217074
 C,-0.0880070255,-1.3219196198,-0.6395973994
 C,5.6645473939,-1.8902259634,-0.8669190399
 H,5.6850914655,-2.9362819461,-0.5656140477
 C,-3.0229261172,-3.0598905092,-0.036748162
 C,4.4637455829,0.1813803613,-1.2085743495
 C,5.6476379828,0.7532080889,-1.701715766
 H,5.6492019885,1.7864194462,-2.045409032
 C,6.8443944784,-1.3059875896,-1.3187804322
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 C,-4.3831706828,-5.0874837689,-0.2142526608
 C,-4.2332854467,-3.7521104408,0.1501757648
 H,-5.085688891,-3.2342607382,0.5870539409
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 H,-4.2057808321,4.079599544,-1.0421963967
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 H,-4.1080629162,6.5346586267,-0.88054441
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 C,-3.7615064613,2.6045053222,1.8462764157
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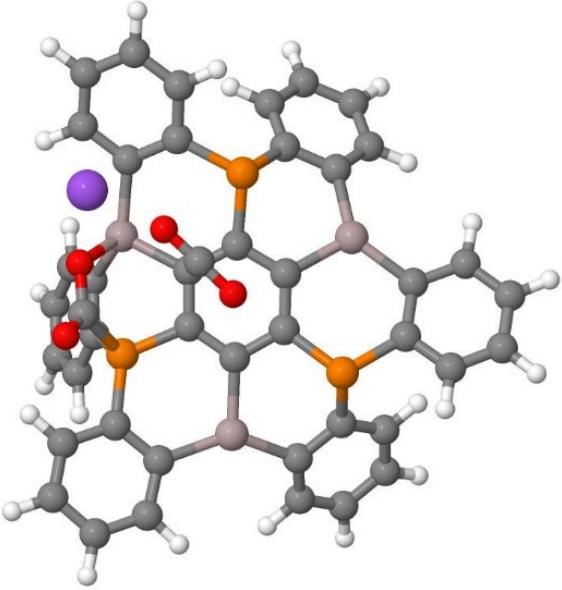
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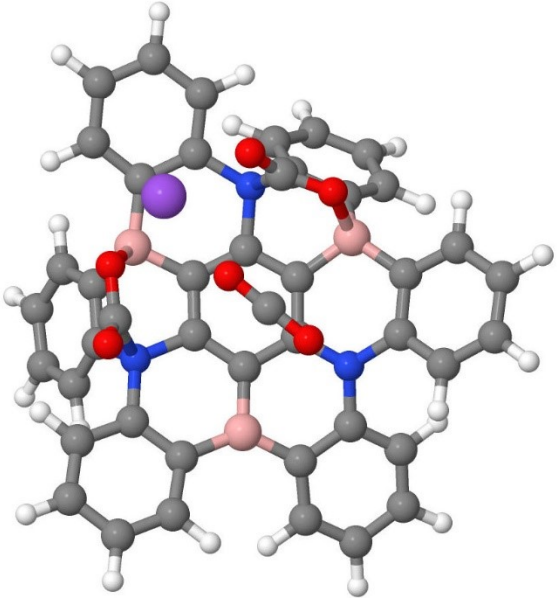
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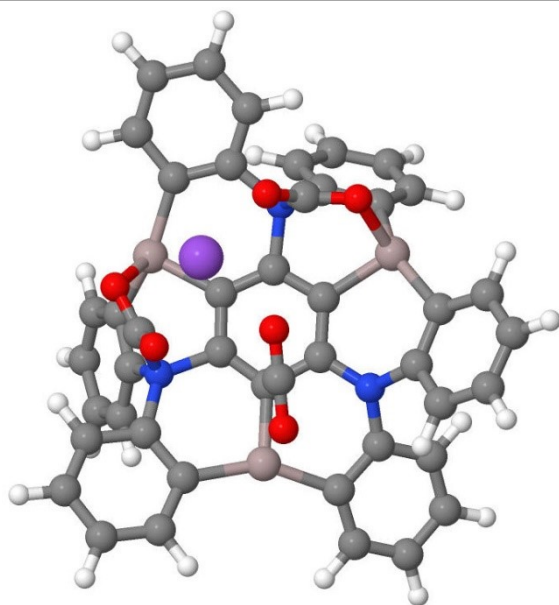
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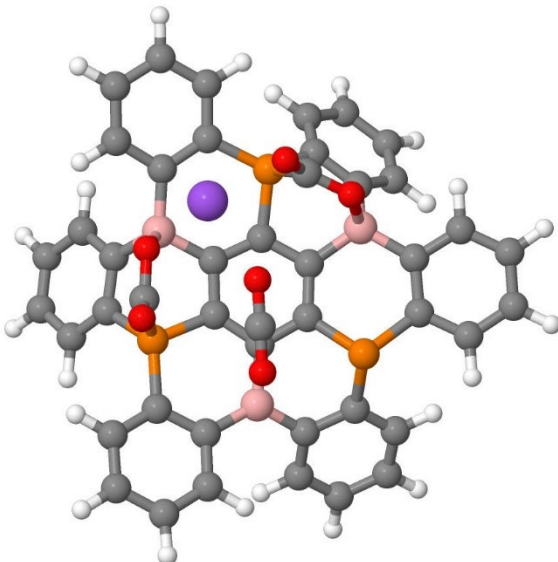
	<p> H,0.4944599882,-5.5893634724,-0.6280527517 C,2.3896029948,5.6052234852,-0.7922890304 H,2.3026926618,6.6424018916,-1.0993418577 C,0.0758374177,-1.4390511966,0.2211681696 C,-5.9623042858,0.5141925275,-1.0858541281 C,-3.5550351001,-0.6992703065,-0.3892968876 C,-3.6007635519,0.7062508692,-0.4494104662 C,-4.8376088026,1.2799177186,-0.8033489537 H,-4.9012007684,2.3653686499,-0.8524915622 C,-4.6710523572,-1.4826006294,-0.6954276085 H,-4.5967590708,-2.5664818321,-0.6788604841 C,-5.8735355918,-0.8784607908,-1.0334370404 H,-6.7357343037,-1.4953757994,-1.2652388531 N,-2.3054944515,-1.4755615335,-0.1200807897 C,-1.0906309684,0.6949223344,0.1138934024 C,-2.2192890322,2.8337329802,0.8376113585 C,-3.4970620278,-2.5595195501,1.8469782866 H,-4.318150462,-1.8557065597,1.7797541591 C,-2.4175994126,-2.5267341034,0.975898123 C,-1.064533172,-0.6763402082,0.1329729299 C,-3.1519462628,3.3258995059,1.7480327523 H,-4.1574315934,2.9119732512,1.7566491966 C,-1.3114620865,-3.3775906499,1.0841918971 C,-0.9338283053,3.3861114954,0.873330699 C,-0.5426117634,4.3539695576,1.7857967604 H,0.4704019755,4.736273379,1.8231420834 C,-2.8023585529,4.3231667864,2.6606792883 C,-3.4929283308,-3.5333477435,2.8483213584 H,-4.3258724268,-3.579843237,3.5423579664 C,-2.4314166675,-4.4269978143,2.963405558 C,-1.3438188616,-4.3390910621,2.0928062859 H,-0.4975207179,-5.0120338317,2.2056956224 C,-1.5038266811,4.8235551306,2.6846399997 H,-1.2222869271,5.5805349749,3.4093478166 C,4.9606892633,1.0339600283,1.5645081074 H,5.0991080729,2.1104956103,1.5722952037 H,4.3580770098,-2.7693685875,1.8138155972 H,6.3418548918,-1.7761456133,2.83942774 O,0.0078769311,3.1630859078,-2.5095142168 C,-0.6399675104,2.7764366632,-1.592936703 O,-1.8307551711,2.2813979868,-1.5715675947 O,-0.9502678834,-3.0391546657,-1.363208932 C,-1.8549070134,-2.1961157102,-1.5266346733 O,-2.3923915376,-1.7491292748,-2.5131695489 O,2.138829764,-0.8846290334,-2.6584593689 C,1.0781009063,-0.4389354506,-2.749466702 O,0.0051825451,0.019320885,-2.8605938361 H,-6.9000716884,0.9927783305,-1.3507055593 H,-3.5386028564,4.6978312426,3.3649778665 H,4.5450174329,5.6038087684,-0.7662617209 H,6.7539640569,0.6800324717,2.6919044262 H,2.6684576004,-6.5660645153,-1.3087680133 H,-2.4426429428,-5.1803161253,3.7450833569 B,2.676715197,1.3807381584,0.3903436275 B,-2.3182740342,1.6151356738,-0.1862308512 B,-0.1243865557,-2.9932186355,0.0872861888 Na,-2.3184206896,0.4677897175,-2.9991336021 </p>
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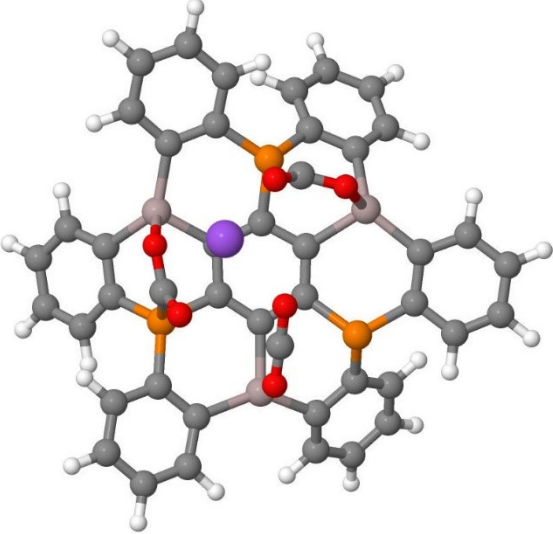


2CO₂-Al₃N₃-NG-Na:CO₂

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 C,3.5722055523,-2.941311178,2.0131511314
 C,4.7672019676,-2.9131221742,2.7169823676
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 C,1.8489360322,-3.325346623,-0.2314706798
 C,0.9616045941,-1.0515479362,0.3820256577
 C,4.3297222393,3.3775762243,-0.5853511162
 H,5.3043523948,2.9150738699,-0.4469614536
 C,0.6841709658,-4.1342744782,-0.2876323972
 C,1.9494810776,3.2871231981,-0.4570279587
 C,1.8753478777,4.5882518428,-0.960186107
 H,0.9097223041,5.075752435,-1.083837081
 C,4.2771886123,4.6730380327,-1.0823526217
 C,3.0882398384,-4.9886215768,-1.5079835589
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 C,1.9675157536,-5.816546258,-1.5407327044
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 H,-0.0883321229,-6.0106741145,-1.0120627998
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 H,-5.2215530335,3.0685040296,-0.8076687622
 C,-4.9949270817,-0.7648163875,-0.9758221214
 H,-4.9448064888,-1.8515925403,-1.0077116738
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 H,-7.0180335791,-0.7174055113,-1.6746483749
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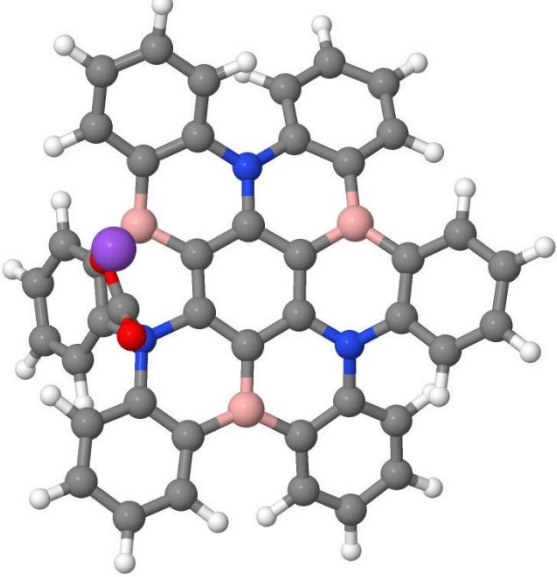
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	<p>2CO₂-B₃P₃-NG-Na:CO₂ E=-3440.61499017H; FreqIm=0 C,-1.3253460122,5.7747248876,-2.3780500748 C,-1.9769242882,3.6431698532,-0.6698492346 C,-0.6058391082,3.9795325496,-0.8794419699 C,-2.9812273114,4.384470855,-1.2896703773 C,-2.656557482,5.4367578686,-2.1469061112 P,2.8978421568,0.947318922,-0.0638590791 P,-2.3257332046,2.3292006638,0.5740869164 C,0.185874472,1.5541575668,-0.2198950161 C,2.0108353881,3.5637684988,-0.0198092716 C,1.177311669,0.5791382844,-0.3280669076 C,-5.0781976673,2.3747345255,0.6086598512 H,-4.946119764,3.4497471855,0.7106334743 C,-3.9661148855,1.5448672269,0.3912057276 C,-1.1481428651,1.1045754597,-0.0535685819 C,2.2457608838,4.9188242524,0.2577018229 H,1.4121910521,5.6135186245,0.2148838825 C,-4.1156401381,0.1375426222,0.3661763727 C,3.1372213655,2.7043585008,0.1161055233 C,4.4040701439,3.1702034942,0.4731946822 H,5.2375111638,2.4794561314,0.5815712539 C,3.5067519523,5.3972626868,0.6176385658 B,0.5395032219,3.0741548722,-0.3423171162 C,-6.3529836012,1.8399828185,0.7505894707 H,-7.2030919357,2.4978484653,0.9043495478 C,-6.5208086383,0.4564419312,0.7388947098 C,-5.413326757,-0.3657651065,0.5604067886 H,-5.553940566,-1.4451428078,0.578282827 C,4.5905461825,4.5294766156,0.7157195269 H,5.5707211212,4.900426033,0.9971858066 B,-2.9266015934,-0.9102245372,0.1461252197 C,-1.4634502514,-0.2537485787,-0.1250013946 C,2.6731240545,-5.6078516857,0.6160838085 C,0.5454518525,-3.9077084612,0.1193424891 C,1.8465921932,-3.3468340804,0.1418793947 C,2.8916528289,-4.2466047194,0.4130357309 H,3.9084790848,-3.8615812391,0.4594017374 C,0.3103442679,-5.2752371823,0.3287110712 H,-0.7051225848,-5.6660916064,0.3225506934 C,1.3797106526,-6.1296094285,0.5655147019 H,1.2054129996,-7.1890924967,0.7228275142</p>

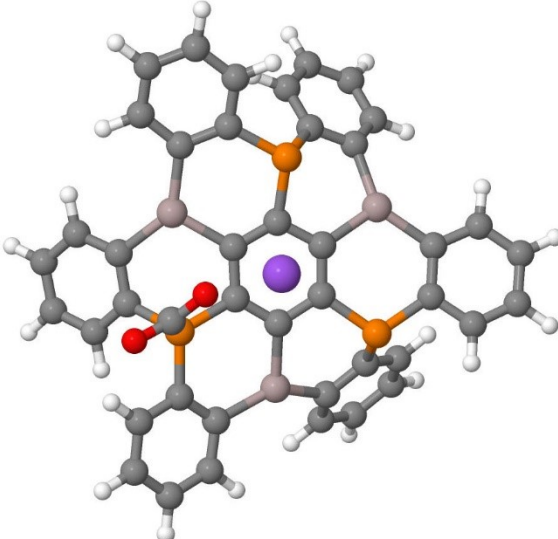
	<p>P,-0.88121897,-2.8374367199,-0.0179955167 C,0.950709328,-0.8014869381,-0.3217838345 C,3.4006827944,-1.4249650001,-1.1256269339 C,-2.3782843194,-4.1902547287,-2.0065786489 H,-1.6160528055,-4.9624616585,-2.073539634 C,-2.2673127688,-3.1410886846,-1.0948482854 C,-0.3886493417,-1.1453337451,-0.291787547 C,4.0116558215,-2.3066730019,-2.0207257751 H,3.7060491413,-3.3499244749,-2.0379293857 C,-3.2031281189,-2.0910388854,-0.960092228 C,3.8365401675,-0.081031035,-1.192876919 C,4.8256032029,0.3757083016,-2.0607968568 H,5.1181615898,1.4226561623,-2.0775610403 C,5.0061284905,-1.8749758778,-2.9028003563 B,2.2103872387,-1.7844910242,-0.0733405667 C,-3.4862342011,-4.208605249,-2.8480019538 H,-3.6080481654,-5.0100773697,-3.5694817561 C,-4.4255789387,-3.1795030788,-2.7695849276 C,-4.2842299209,-2.1400432129,-1.8481629643 H,-5.0278835958,-1.3485755834,-1.8238477638 C,5.4193850359,-0.5436618077,-2.9232456065 H,6.1914019723,-0.2195453908,-3.6135302056 C,-0.3188999249,5.0520904736,-1.7453574844 H,0.7180980799,5.3020962196,-1.9568749093 H,-4.0249462008,4.1240785098,-1.1442427576 H,-3.4514005007,5.9841958109,-2.6452640145 O,3.273830791,0.4928099801,2.6169631408 C,3.038472108,-0.0283871985,1.5562284034 O,2.7253563739,-1.2914458962,1.371977625 O,-2.6707108581,-1.6949625927,1.5581832471 C,-1.6403696487,-2.4365658889,1.6688953135 O,-1.0402419939,-2.7777170115,2.6824454953 O,0.5645203917,2.4000734538,2.8374246492 C,0.4037307524,1.2560313466,2.8398280045 O,0.2460616694,0.0956710424,2.8398479354 H,3.5137742504,-6.2658951531,0.8158800402 H,5.462448743,-2.5868275906,-3.5843394051 H,3.6394324979,6.4537318819,0.8300186403 H,-1.0746286689,6.5882600709,-3.0513484967 H,-7.5055724716,0.0228270829,0.8858556924 H,-5.2803152481,-3.1853568121,-3.4397479307 Na,1.1129551691,-2.0947791923,2.922301541</p>
	<p>2CO₂-Al₃P₃-NG-Na:CO₂ E=-4093.29532338H; FreqIm=0 C,-1.9708713189,5.9975552484,-2.3365817311 C,-2.2177942933,3.7144879199,-0.7226897174 C,-0.9844341885,4.4199695166,-0.7568939956 C,-3.2881642421,4.1438671317,-1.5085793348 C,-3.1632772343,5.2819721777,-2.3089195676 P,2.9137642837,0.9387006175,-0.1126852016 P,-2.3430183268,2.3128073721,0.4931635255 C,0.1686495327,1.5123866752,-0.3012136797 C,2.4681576423,3.7337432733,0.1236458375 C,1.1644944908,0.5540419194,-0.4883912796 C,-5.0157072216,2.7646250897,0.7773267396 H,-4.6779737959,3.7953997515,0.8665207298 C,-4.0936811726,1.7387877221,0.50368304 C,-1.1752250774,1.047285104,-0.2169440357 C,2.9918368971,5.0099026286,0.3854182722 H,2.3382936874,5.877922601,0.3257380303 C,-4.524492792,0.3909367235,0.4719199951 C,3.3738433322,2.6522152194,0.2210450839 C,4.7135894196,2.8363018194,0.5943764157</p>

	<p> H,5.3903979541,1.9881885403,0.6786838003 C,4.3258255698,5.2077185864,0.7394498481 Al,0.5480742659,3.4264219394,-0.1175424497 C,-6.3672072946,2.4852959074,0.9455831325 H,-7.0634371981,3.2950486697,1.1433319462 C,-6.8178577831,1.1683796467,0.874574488 C,-5.8987376478,0.1473158604,0.6536607158 H,-6.2647164077,-0.878590631,0.6318613756 C,5.1863886687,4.1176458606,0.8561209994 H,6.2216662755,4.2616779773,1.1483419323 Al,-3.2685889799,-1.068439875,0.1980050792 C,-1.4841395479,-0.3153562457,-0.2923445764 C,2.2211873033,-6.2860097032,0.3940649625 C,0.432898717,-4.1852558341,0.0556836962 C,1.8151099464,-3.9085753256,-0.0528582632 C,2.6831486577,-5.0005074871,0.1173946929 H,3.7578432199,-4.845027382,0.0396992585 C,-0.0432047009,-5.4711269751,0.3570251384 H,-1.1097397977,-5.6589835612,0.4619901643 C,0.8536263459,-6.5203685615,0.5246686992 H,0.4839676981,-7.5141188049,0.7569181741 P,-0.8641485679,-2.929661111,-0.080437092 C,0.9460821544,-0.8421802949,-0.5694896614 C,3.956718003,-1.3048190515,-1.3461519327 C,-2.17788359,-4.5564067981,-1.937740814 H,-1.256465754,-5.1264038622,-2.0209859409 C,-2.2813535007,-3.4614153601,-1.0714574182 C,-0.394035924,-1.201862892,-0.4743252638 C,4.8329844481,-1.9226812467,-2.2468403877 H,4.7999331303,-3.002808286,-2.3715716514 C,-3.4482474983,-2.6705343791,-0.9604969882 C,4.0571824803,0.1040232962,-1.2455871556 C,4.9579179848,0.8569512199,-2.0077194006 H,4.9976920782,1.93970844,-1.9269595749 C,5.7507083597,-1.1912166968,-3.0028262204 Al,2.4761709128,-2.0801298284,-0.2959410868 C,-3.2815293064,-4.9049430099,-2.7106902227 H,-3.2201789889,-5.7512704838,-3.3876574593 C,-4.4572273813,-4.1610145912,-2.6162513416 C,-4.5299115114,-3.0598978153,-1.7620086683 H,-5.4539761497,-2.486763493,-1.7275181154 C,5.8090097065,0.1964594357,-2.8898611044 H,6.5121485985,0.7669520475,-3.4883705077 C,-0.8863991593,5.5505558733,-1.5802096566 H,0.0512979078,6.1011122698,-1.6381315913 H,-4.2248667821,3.594370758,-1.5109577964 H,-4.0052164942,5.6031498948,-2.9154600888 O,2.6664847766,0.5716654251,2.5622775481 C,2.8829688252,-0.0302343207,1.5224448588 O,2.8644392613,-1.3205641596,1.409004341 O,-2.5894718968,-1.9354422848,1.7592332487 C,-1.4383379153,-2.4657121019,1.6830310091 O,-0.5913098803,-2.5767128597,2.5654013033 O,0.4194722627,3.0044612078,2.3750130617 C,0.116146903,1.9234518027,2.6902782504 O,-0.1671664246,0.8445143463,3.0158428239 H,2.9262001158,-7.1027557918,0.5180167066 H,6.4176870501,-1.7043304751,-3.6895137405 H,4.6921275549,6.2107963812,0.9366797043 H,-1.8799704851,6.8880022384,-2.9512956569 H,-7.8711205288,0.940758917,1.009371636 H,-5.3175502285,-4.4360583248,-3.2197757811 Na,1.1359195665,-1.292066148,3.1562458866 </p>
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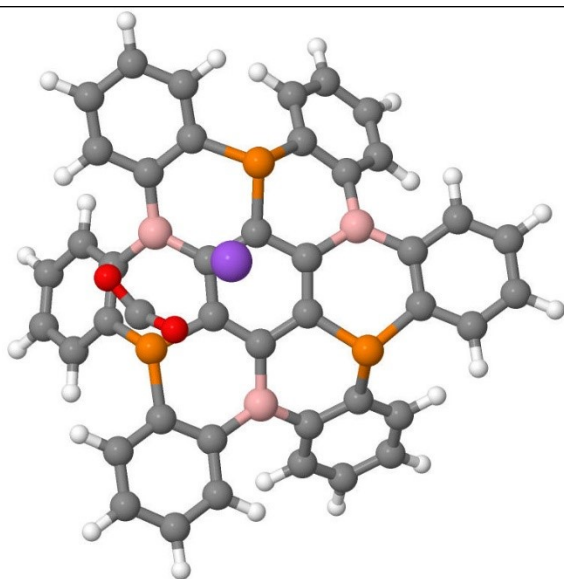
Table S7: Geometries, energies (in Hartree) and Cartesian coordinates (in Å) of the transition states with a Na⁺ cation in vacuum. Level of theory: M06-2X/6-311++G*//M06-2X/6-31+G*

	<p>B₃N₃-NG-Na/CO₂ E=-2203.83031345H; FreqIm=1</p> <p>C,1.1657673404,-5.8625599535,-1.7197350025 C,1.7936702224,-3.3693659168,-0.5868886332 C,0.4527823505,-3.825213148,-0.56956038 C,2.7890906092,-4.1415443406,-1.2048972888 C,2.475889509,-5.3747155609,-1.7553316422 N,-2.5055373499,-0.5467863963,0.0722377956 N,2.1487897489,-2.0883528872,-0.0604797015 C,-0.1604303846,-1.3920826655,-0.1089312266 C,-2.1320515708,-3.0453776915,0.2287615554 C,-1.0404694155,-0.3348990506,-0.1193252339 C,4.1238121907,-2.9329443026,1.0962576944 H,3.6571377538,-3.909511718,1.1593434254 C,3.4516692006,-1.8641550709,0.4795498207 C,1.2271939664,-1.0581250348,-0.0912330203 C,-2.6772416244,-4.2893835584,0.5983623481 H,-2.0390088806,-5.1670787774,0.5718024756 C,4.024119644,-0.5712795738,0.4783587395 C,-2.975414704,-1.9338852559,0.3435017305 C,-4.2885105786,-2.038089011,0.8014591466 H,-4.9132564688,-1.1521842887,0.8866183379 C,-3.9869525061,-4.4192141519,1.0405148086 B,-0.6341056616,-2.8337489687,-0.1309345834 C,5.3737900081,-2.7366582071,1.660132142 H,5.8722995686,-3.5715533147,2.1434384363 C,5.9775806969,-1.4744512933,1.6389415194 C,5.295531472,-0.4143697419,1.0680125677 H,5.7299764893,0.5805195364,1.1089047572 C,-4.796082026,-3.2866905542,1.1395921555 H,-5.8188716963,-3.3701531316,1.493222019 B,3.1453800857,0.6066676278,0.0211969001 C,1.6686596685,0.2790556392,-0.0605833673 C,-1.6596850838,5.7013568096,0.8400476704 C,0.162608475,3.6567984473,0.1769745041 C,-1.2197555136,3.4872390809,-0.0928029658 C,-2.1041147958,4.5356858478,0.2367899517 H,-3.1636188641,4.3986056957,0.0299709762 C,0.6026054433,4.8232922674,0.8260118946 H,1.6493368062,4.9367375424,1.0869010878 C,-0.2987732451,5.8274302226,1.148191127 H,0.0631730646,6.7178783991,1.653797224 N,1.1042868602,2.6384418203,-0.1476420593 C,-0.6743345255,1.0103921475,-0.1856325705 C,-2.9779100489,1.5376923022,-1.184289796 C,2.67826501,4.2243318879,-1.1405686865 H,1.8597201237,4.9080081279,-1.3347071417 C,2.4416556525,2.9834418303,-0.5285925461 C,0.7038243045,1.3099455995,-0.1284716498 C,-3.714404795,2.2375861882,-2.1410804923 H,-3.490792395,3.2877293678,-2.3126916507 C,3.4964317001,2.0544204968,-0.3773163396 C,-3.2764449962,0.173836492,-1.0004100176 C,-4.2299044795,-0.4794137757,-1.7628086499 H,-4.4300214498,-1.5370125618,-1.6440835036 C,-4.698883592,1.6058380214,-2.9040679672 B,-1.6944257129,2.0859292633,-0.4962712185 C,3.9596655898,4.5714272633,-1.5416870332 H,4.1200166428,5.531157308,-2.0236701658</p>
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	<p>C,5.0272704094,3.6874180515,-1.3633124716 C,4.7808669092,2.4435840296,-0.8061549102 H,5.5914725661,1.724052662,-0.7354753229 C,-4.9387106134,0.2502998922,-2.7246938172 H,-5.6777628086,-0.2612282139,-3.3330064838 C,0.1766577382,-5.0823516404,-1.1468095929 H,-0.8529587608,-5.4256961649,-1.183620677 H,3.8029061491,-3.7646832689,-1.2791052556 H,3.2583692193,-5.9497197783,-2.2413296631 O,-3.5538784201,1.1137277879,1.5356486764 C,-2.733806258,0.2064100887,1.5578657866 O,-1.9837270144,-0.238637783,2.4120263959 H,-4.3744179542,-5.3927989747,1.3232569888 H,0.924661952,-6.8218966208,-2.1657593494 H,6.9522616423,-1.3252140981,2.0922090667 H,6.0255569398,3.9587336055,-1.6910471832 H,-2.3536237848,6.4991719592,1.0852660597 H,-5.2577674902,2.1655223984,-3.6473622795 Na,-2.3051012542,1.885900739,3.2997777546</p>
	<p>B₃N₃-NG-Na/CO₂ (2) E=-2203.82404616H; FreqIm=1 C,-0.1051516936,-6.0037083652,-1.5624771298 C,1.0396998559,-3.6864657131,-0.4515831214 C,-0.3708155615,-3.8415937716,-0.4445480616 C,1.8483513495,-4.6707123666,-1.046824145 C,1.2813705162,-5.8134216063,-1.5845786773 N,-2.5880054985,0.0098121002,0.1381178801 N,1.6590585691,-2.5064891577,0.0503763159 C,-0.4544687607,-1.3438739584,0.0460526344 C,-2.7552871505,-2.5179831242,0.2724820756 C,-1.0793543333,-0.1063418629,0.0360409217 C,3.4497697133,-3.7051776939,1.1953103647 H,2.7896330269,-4.5580859366,1.3086669958 C,2.9975118607,-2.5416225551,0.5524674331 C,0.9643832608,-1.3064973011,0.0348765152 C,-3.5858736284,-3.6175375802,0.5662041497 H,-3.1494710949,-4.6109416987,0.5762400399 C,3.8275402068,-1.3991316533,0.4849757704 C,-3.3544434631,-1.2560909026,0.3481282943 C,-4.6990989009,-1.0823292611,0.6684074042 H,-5.1287869094,-0.0845821795,0.7171343446 C,-4.928881469,-3.4689209151,0.8824385639 B,-1.2254905479,-2.642163546,-0.0142122236 C,4.7332402712,-3.7597491085,1.7158032046 H,5.0618751879,-4.6644649286,2.2185148963 C,5.5878221103,-2.6561944154,1.6249265936 C,5.1233568493,-1.4947076386,1.0311348959 H,5.7582900595,-0.6131019628,1.0189578238 C,-5.4917478972,-2.1920574035,0.9238707953 H,-6.5401088518,-2.058542849,1.1706813115 B,3.1939214707,-0.0733446973,0.0197256691 C,1.677994876,-0.0875991598,0.0174105725 C,-0.3643287433,5.9630665535,0.8848994152 C,0.9186496912,3.546201309,0.2197484412 C,-0.4810327874,3.6708374989,0.049934344 C,-1.0888423755,4.8956234793,0.3727117515 H,-2.1641738175,4.9880694767,0.2306533317 C,1.6394468991,4.6054279239,0.7929029178 H,2.699900312,4.4942313772,0.9914320058 C,1.0042290683,5.7975015973,1.1152095131 H,1.5852428569,6.6029343035,1.554645503 N,1.6162713461,2.3405791357,-0.1257344206 C,-0.4513878004,1.1156241852,-0.0390779656</p>

	<p>C,-2.5074354496,2.089596953,-1.2153056535 C,3.4330789037,3.5339423112,-1.243653412 H,2.7689089592,4.3722969205,-1.4197799673 C,2.9680795836,2.3854468712,-0.5808349613 C,0.9559802042,1.1224251772,-0.0438378031 C,-2.9493043427,2.8672971401,-2.2845833183 H,-2.5043840703,3.8466383379,-2.4421830677 C,3.8129409477,1.2569150924,-0.4473933441 C,-3.0931851053,0.8272902465,-1.0456837108 C,-4.0408510429,0.3156458913,-1.919175684 H,-4.4534403121,-0.6789939931,-1.8058096274 C,-3.9236321822,2.391736875,-3.1641874177 B,-1.2919701529,2.3894774504,-0.2661713388 C,4.7354483202,3.5904536729,-1.7140381244 H,5.0695824946,4.4828737774,-2.2349044922 C,5.6023890804,2.5045941275,-1.5543539931 C,5.1284241266,1.3558201992,-0.9451916629 H,5.7719378078,0.482636525,-0.8839128986 C,-4.4516943483,1.1177017634,-2.9884383166 H,-5.186261648,0.7276119732,-3.6854840691 C,-0.9049526997,-5.0188724768,-1.0139308713 H,-1.9834429414,-5.1314549002,-1.0647064528 H,2.9197534705,-4.5234649282,-1.118213566 H,1.9253050489,-6.5510327364,-2.0541436452 O,-2.4983307717,2.0803883279,1.3670799222 C,-2.7010194008,0.8536943918,1.4934243212 O,-2.8843936576,0.2065571167,2.5106106718 H,-5.5366426925,-4.339926167,1.1062411274 H,-0.5449103175,-6.8931920376,-2.0016556926 H,6.5883655992,-2.7014414626,2.0428772305 H,6.6175159498,2.5513482359,-1.9350410803 H,-0.8520402154,6.9037481145,1.1207914056 H,-4.2535972203,3.0059149882,-3.9962334368 Na,-2.3327739979,2.1552375938,3.6280819851</p>
	<p>Al₃N₃-NG-Na/CO₂ E=-2856.39777560H; FreqIm=1 C,-4.3227449419,-4.5092243783,2.0105563741 C,-3.2526747555,-2.2174522206,0.7642520515 C,-2.5083128407,-3.4249267822,0.7706067614 C,-4.4978292459,-2.1747487228,1.4141768121 C,-5.0249260532,-3.3026962299,2.025899665 N,2.0746552671,-1.5609035473,0.2523919782 N,-2.8610822638,-0.9929812627,0.095328781 C,-0.4427177605,-1.3355758948,0.2267257423 C,1.0724356775,-3.899572212,-0.1725576754 C,0.8260622305,-0.7521409957,0.2674295442 C,-4.6938313734,-1.235277751,-1.4563248481 H,-4.4344261506,-2.2894559596,-1.4978423936 C,-3.9296725471,-0.3679703564,-0.6562839511 C,-1.5531605583,-0.4486882985,0.1676854854 C,1.3615641565,-5.2140496907,-0.5936134068 H,0.5675600208,-5.9575384514,-0.584370843 C,-4.2601467437,1.0092783952,-0.6052475756 C,2.1266327968,-2.9638448906,-0.2012333893 C,3.4043588823,-3.3536511008,-0.6249383418 H,4.2207840062,-2.6334809662,-0.6022148976 C,2.6255503949,-5.6000335215,-1.017432469 Al,-0.6702032839,-3.2128082142,0.2823792037 C,-5.7892545457,-0.7685392404,-2.1696290503 H,-6.3624947091,-1.4608707769,-2.7790774227 C,-6.1501946675,0.5784361046,-2.1055818071 C,-5.3785968568,1.4448884596,-1.3425092232 H,-5.650555553,2.4978569664,-1.3155105437</p>

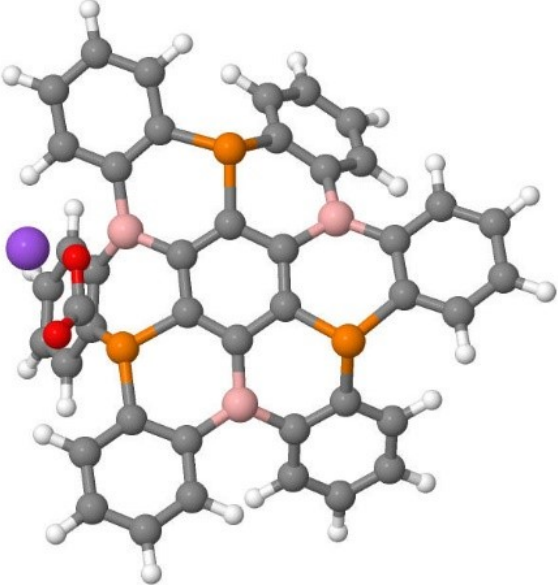
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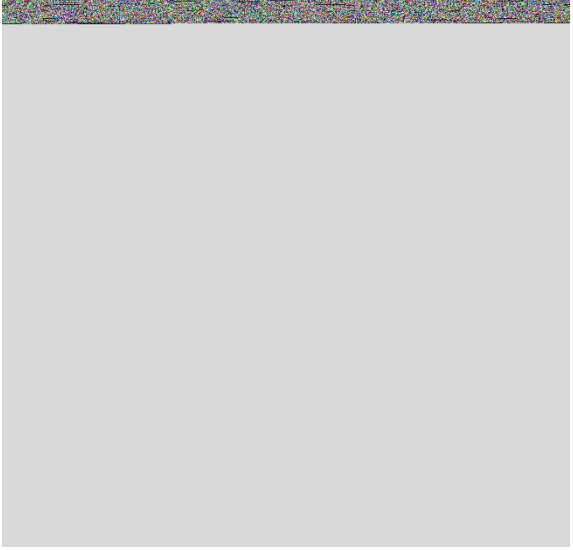


B₃P₃-NG-Na/CO₂

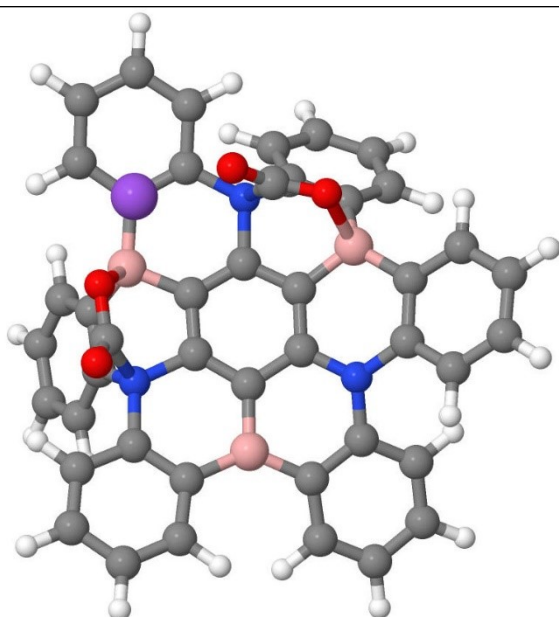
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 C,4.0858887609,-3.1468882787,-1.1148727634
 C,4.0355439532,-4.1325816785,-2.101902643
 P,-2.4941202812,-1.6640449482,0.352020018
 P,2.9477853679,-1.5828053807,0.9598322805
 C,0.2847687236,-1.463650442,0.355060386
 C,-0.8794633002,-3.9206598995,0.172629365
 C,-0.9231642543,-0.7932495149,0.2442983356
 C,5.6007056358,-0.8939663707,1.0294401474
 H,5.7521792265,-1.956463106,1.2088856446
 C,4.3135871364,-0.4016093617,0.7730163379
 C,1.4517076966,-0.6595242291,0.5441550748
 C,-0.7153440914,-5.3117246972,0.2835402531
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 C,-1.9039147654,5.0190695541,0.9278825534
 H,-1.1163989719,5.6696046027,1.3032425932
 C,-3.1952779181,5.5207280103,0.8010056622
 H,-3.3953048444,6.5617646097,1.0364052047
 P,0.0473439928,3.0948669601,1.0394665602
 C,-1.0719904295,0.6198116832,0.3010036727
 C,-3.3831936243,0.4686821422,-1.0613230088
 C,1.0924258213,4.9723787045,-0.7954107709
 H,0.1773633811,5.5396229229,-0.6534429221
 C,1.2875093949,3.7595431964,-0.1377879899
 C,0.0964488216,1.3558089298,0.5364035045
 C,-4.0971924309,1.0658111851,-2.1093044349
 H,-4.0169347276,2.1379514414,-2.2652908134
 C,2.4747650918,3.0057566027,-0.314514284
 C,-3.4872677064,-0.9399530136,-0.9570085933
 C,-4.2864534793,-1.7014448417,-1.8043662896
 H,-4.3401611183,-2.7816713849,-1.696655974
 C,-4.8919348045,0.3146367657,-2.9776543591
 B,-2.4161615101,1.3122635831,-0.1340780334
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 H,1.8887792972,6.37695683,-2.2147940611
 C,3.2116912207,4.7021924329,-1.9196817826
 C,3.4117468193,3.5040773073,-1.2386350531
 H,4.3059103547,2.9249303048,-1.4506620352
 C,-4.9978204849,-1.0638590728,-2.8213580017

	<p>H,-5.6167181709,-1.6469941646,-3.4959016535 C,1.6884008117,-4.4439641664,-1.6780547061 H,0.752174156,-4.9363499291,-1.9282926825 H,5.0241401468,-2.6352022421,-0.921510318 H,4.9360845279,-4.3814608757,-2.6556534873 O,-3.7863185441,0.0245849192,2.007608001 C,-2.9687172204,-0.871516433,2.1000302935 O,-2.1812999082,-1.2614033598,2.9792355525 H,-1.6259873665,-7.2368561203,0.5845336434 H,2.7965190354,-5.5381746145,-3.1650587147 H,7.3320957004,2.025682855,1.0695941178 H,3.9523737513,5.053276227,-2.631343372 H,-5.2517984555,5.0480798271,0.3595514918 H,-5.4281839571,0.8108520789,-3.7807254408 Na,-0.8264173163,0.4707601539,3.1653194495</p>
	<p>B₃P₃-NG-Na/CO₂ (2) E=-3063.53948693H; FreqIm=1 C,-3.1669755038,-4.7242533885,2.1115201337 C,-3.1463653302,-2.6732628759,0.2019358947 C,-1.940827605,-3.3722952261,0.4814702532 C,-4.3324939163,-3.0246220974,0.8449288137 C,-4.339985027,-4.0400579631,1.8012608954 P,2.299182351,-1.6557597928,-0.1193366826 P,-3.1021766052,-1.4231858449,-1.145680454 C,-0.443312819,-1.4036897961,-0.4970977842 C,0.6743598746,-3.8730393359,-0.2079036443 C,0.775050965,-0.748817745,-0.3394693617 C,-5.7305423161,-0.6356113039,-1.2076568995 H,-5.9138238127,-1.6781645343,-1.459990749 C,-4.4305312054,-0.2043248059,-0.9095236964 C,-1.5771469916,-0.5643794621,-0.6894892391 C,0.5021887893,-5.2558007013,-0.3794910153 H,-0.5055949613,-5.6574842788,-0.4344117362 C,-4.1690610704,1.1661592412,-0.6555529128 C,2.0139377567,-3.4126900694,-0.191943204 C,3.109896428,-4.2709146804,-0.309533918 H,4.1233030571,-3.876705713,-0.3109308974 C,1.5864704674,-6.1241171635,-0.5047303812 B,-0.5806658989,-2.9153768262,-0.1231625435 C,-6.7915121673,0.2634744421,-1.2252677266 H,-7.7949894528,-0.0886909214,-1.4452882717 C,-6.5531463419,1.6196774055,-1.004062099 C,-5.2616261745,2.0545799712,-0.7330610098 H,-5.0834131739,3.1178515451,-0.5991180718 C,2.891353831,-5.6382491979,-0.4561924526 H,3.7343139318,-6.3151865788,-0.5506158395 B,-2.7367606352,1.7109419308,-0.3708000526 C,-1.4702913294,0.8344514571,-0.6736565161 C,4.2375664484,4.6273681032,-0.1945781828 C,1.6104899649,3.6934658582,-0.523306698 C,2.6282432282,2.7826472167,-0.1556884319 C,3.9350228958,3.2837204019,-0.0070941486 H,4.7316977839,2.5922139188,0.261669316 C,1.925394292,5.0457792379,-0.731703738 H,1.1527128108,5.73625596,-1.0646574168 C,3.2208802748,5.5159530252,-0.5477433338 H,3.4410127115,6.5684679125,-0.7000536607 P,-0.0839089824,3.1891865784,-0.9956444948 C,0.9665534224,0.6452149501,-0.3722887365 C,3.068997168,0.4821262223,1.2836759218 C,-1.0247444276,4.9096996519,1.0597735155 H,-0.0915578298,5.4571564424,0.9615203081 C,-1.2633654478,3.7720824869,0.29089419</p>

	<p>C,-0.1730191072,1.4180335419,-0.607215543 C,3.627139571,1.1279002006,2.3926075215 H,3.6178997304,2.2135606688,2.4370420174 C,-2.4785460755,3.0500259526,0.4113810086 C,3.0812612316,-0.9301348634,1.3213591524 C,3.6332886895,-1.6715690081,2.3616475275 H,3.6157494229,-2.7586542744,2.3440422454 C,4.1784025338,0.4059116008,3.4550107618 B,2.3405131554,1.2669608674,0.0911102589 C,-1.9659944729,5.3288139424,2.0005216452 H,-1.7613851711,6.2031240145,2.6117618572 C,-3.1486001646,4.614982333,2.1711979469 C,-3.3947085467,3.4940376073,1.3822097013 H,-4.3102251193,2.9315010071,1.542983747 C,4.1900159622,-0.9868529807,3.4419446074 H,4.6175996307,-1.540156361,4.2719934033 C,-1.9877407378,-4.3905577254,1.453299937 H,-1.0725694803,-4.9119292635,1.7220956148 H,-5.2523436572,-2.4867915852,0.6351248326 H,-5.2654581558,-4.284441089,2.3147254465 O,3.5052762671,0.2585881468,-1.4776984733 C,3.387818082,-0.9994052735,-1.5197466419 O,3.8938414039,-1.7683260505,-2.3447424022 H,1.4106027164,-7.1865799886,-0.6435269195 H,-3.1710167334,-5.5061906122,2.8643337698 H,-7.3687307586,2.3341598215,-1.0589437421 H,-3.8738460435,4.9264324169,2.9165944722 H,5.2558758557,4.9834656636,-0.0691676893 H,4.5986800164,0.9384014983,4.303005066 Na,4.6745865282,0.1016031356,-3.3978850445</p>
	<p>Al₃P₃-NG-Na/CO₂ E=-3716.14879332H; FreqIm=1 C,-3.2042770925,-4.8964911625,2.5282827845 C,-2.9541468765,-2.9776173201,0.4929961994 C,-1.8605571193,-3.8325038885,0.7896518516 C,-4.142443894,-3.0902428623,1.2171744408 C,-4.2628408184,-4.0458947693,2.2296481383 P,2.662979142,-1.415754053,-0.3716710245 P,-2.8158170073,-1.855187855,-0.9920760035 C,-0.1583013068,-1.432504051,-0.393533213 C,1.633479628,-4.0816676036,-0.0929890406 C,0.9941050351,-0.6645916576,-0.2267950991 C,-5.4743369808,-1.7412029772,-1.4765271151 H,-5.2795747266,-2.7621885052,-1.8009147982 C,-4.4199253102,-0.9439736215,-1.0026735915 C,-1.4004348084,-0.7342572144,-0.5311995914 C,1.8719853109,-5.4658642212,-0.1050741822 H,1.0539981386,-6.1526387766,0.1043125727 C,-4.6701374568,0.3946550779,-0.6182754252 C,2.7321990465,-3.2358509593,-0.3770551681 C,3.9937896807,-3.7612885372,-0.6939579655 H,4.8183181769,-3.0995919479,-0.9467254423 C,3.1287606359,-5.9955213716,-0.3934644667 Al,-0.1505807235,-3.3368627482,0.0417908762 C,-6.7755309997,-1.2499432239,-1.5254047886 H,-7.578625752,-1.8876576769,-1.8826593161 C,-7.0410862162,0.0600445118,-1.1287526772 C,-5.9936951882,0.8675907772,-0.6956934853 H,-6.2127909883,1.896667222,-0.4154922381 C,4.185545993,-5.1412525215,-0.6985868339 H,5.1628650759,-5.5437202951,-0.946163524 Al,-3.1754421887,1.539739492,-0.2099537137 C,-1.4574249775,0.66506204,-0.5310253629</p>

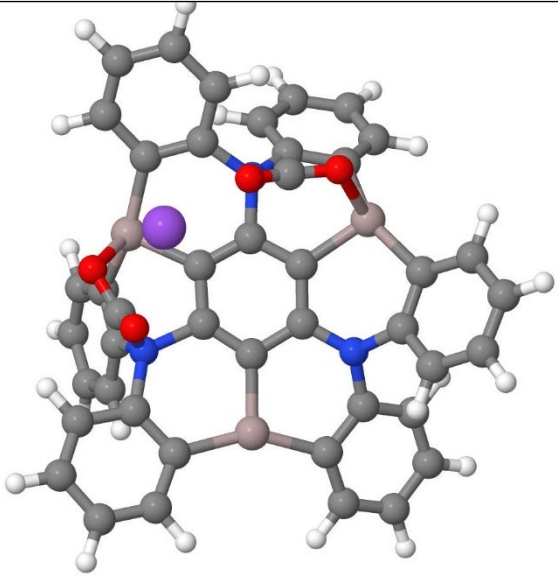
	<p> C,3.2700043938,5.9526286007,-0.2942108313 C,1.1000110418,4.1724989118,-0.4661345035 C,2.3722131385,3.6851971142,-0.0843492443 C,3.4390898138,4.601604517,-0.0122829615 H,4.4315515112,4.2494978601,0.2636881717 C,0.9460769048,5.5316096612,-0.7883155814 H,-0.0222450559,5.9059012732,-1.1169361236 C,2.0144099726,6.4162822136,-0.6868620859 H,1.8689113639,7.4650644503,-0.9279773344 P,-0.4604165598,3.221061217,-0.7173745093 C,0.9972390783,0.7629167913,-0.207479578 C,3.9391165981,0.6480570662,1.0055372021 C,-1.2170423402,4.8032894855,1.5359662951 H,-0.2226982911,5.2377644736,1.5003698239 C,-1.5813817842,3.7762041864,0.6634925552 C,-0.2394295661,1.4026609668,-0.3691370928 C,4.8823948393,1.1277045092,1.9245353303 H,5.0276837869,2.200012324,2.0396227998 C,-2.8784751998,3.2067236813,0.7325765879 C,3.7867305012,-0.757427657,0.9103715795 C,4.5345797962,-1.6277968628,1.704089799 H,4.4032763599,-2.7029996642,1.6325328657 C,5.6484108395,0.264131639,2.7106251509 Al,2.6020893947,1.7954933818,0.177334071 C,-2.131774031,5.2825659222,2.4772955323 H,-1.8333660422,6.0795649807,3.152199665 C,-3.4110828341,4.7437663083,2.5555066807 C,-3.7683427938,3.7040118014,1.6959669033 H,-4.7658549714,3.2762087264,1.7824904364 C,5.4651253037,-1.1100203104,2.606938546 H,6.0447986183,-1.7881084019,3.2256124183 C,-2.0094139925,-4.7743886988,1.8181310267 H,-1.1808019345,-5.4325315567,2.0745394506 H,-4.9844457666,-2.4376849078,1.006886088 H,-5.1931206802,-4.1180592692,2.7856728591 O,4.4739151124,-1.1712715579,-2.3454754113 C,3.3618170344,-0.7566488835,-2.1215444917 O,2.5498143388,-0.0055123348,-2.6978062716 H,3.2795499985,-7.0708474064,-0.3943810725 H,-3.3039998445,-5.6437282707,3.3095524075 H,-8.0532355673,0.4507006456,-1.1720593188 H,-4.1226055869,5.123105976,3.2826040445 H,4.1099515667,6.637064611,-0.2255525026 H,6.3795113283,0.6655157092,3.4058350744 Na,0.4323847749,0.403634477,-2.8076432473 </p>
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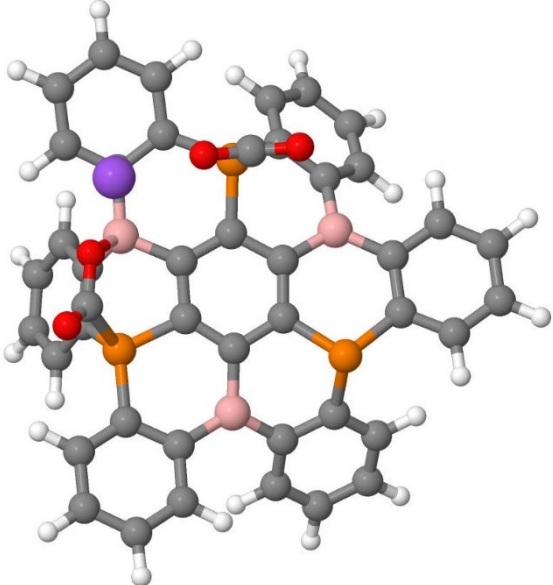


1CO₂-B₃N₃-NG-Na/CO₂

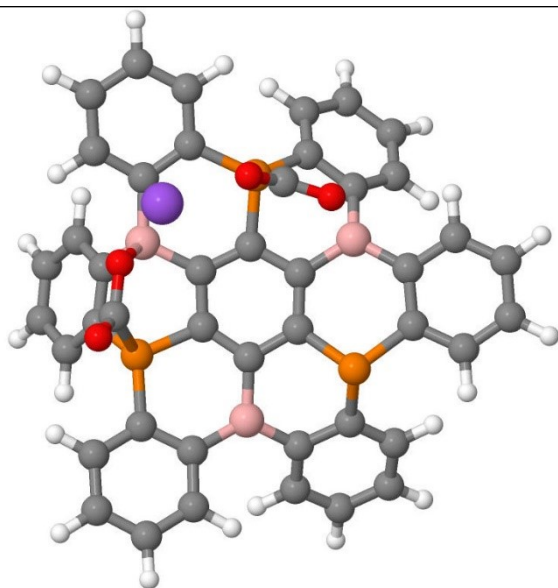
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 H,-2.5598261379,6.4517999892,-1.974961396
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	<p>H,-3.3588270989,4.2640149054,1.1813420225 H,-5.6451115128,4.070091369,2.0207302682 O,-0.9468552726,-3.1037058475,-2.5453850356 C,-0.3126477989,-2.8816999342,-1.5673938958 O,0.9690452334,-2.8297850534,-1.4098945558 O,2.0144637876,2.4947418429,-1.5572629846 C,2.467574771,1.3626482208,-1.6371185317 O,2.7823548788,0.5759059246,-2.4981417574 H,6.0748963623,-3.352541199,-0.7988249381 H,1.1580775956,-5.2771942899,3.7923286795 H,-6.2310246559,-3.6422920596,-1.2787937252 H,-6.8770094298,1.9060879956,1.8642114753 H,-0.1609720566,7.1017520393,-1.7621230777 H,3.8731039907,4.4036490576,3.5174588808 B,-3.1156819161,-0.2713464245,-0.0161910567 B,1.5020391006,-2.257094881,0.0027285255 B,1.0208611723,2.8459291773,-0.0429053734 Na,2.5077498806,-1.6443902523,-2.7581081225</p>
	<p>1CO₂-Al₃N₃-NG-Na/CO₂ E=-3044.92493709H; FreqIm=1 C,-4.7979663613,4.0930034008,1.8323645926 C,-2.414190532,3.1243576755,0.6702011683 C,-3.6225495619,2.3945902701,0.5151033196 C,-2.4227486204,4.302261246,1.4382083738 C,-3.5934580814,4.7791592186,2.0071617526 N,-1.7295379615,-2.2076971946,-0.2341348427 N,-1.1490695836,2.7856440875,0.0636021808 C,-1.5047619752,0.3554690568,-0.0203059364 C,-4.0702438154,-1.1279705391,-0.6065372175 C,-0.9099741733,-0.883800163,-0.037260098 C,-1.2958377681,4.7629788694,-1.3083159579 H,-2.3504087967,4.5256621908,-1.4126952752 C,-0.4669424013,3.9078645706,-0.5617168242 C,-0.6226744496,1.4721144711,0.0523249548 C,-5.4000958074,-1.3838424947,-0.9998276181 H,-6.1247901621,-0.5739527915,-0.9589513594 C,0.9172639882,4.1976861139,-0.4556204663 C,-3.1825124059,-2.2088626385,-0.6825283087 C,-3.5923061496,-3.4702961653,-1.1180772332 H,-2.8903760489,-4.3024133724,-1.1356321738 C,-5.8249702971,-2.6305764248,-1.4401499919 Al,-3.3725059308,0.6081399723,-0.1099041525 C,-0.795478082,5.9140353132,-1.9003585972 H,-1.4635591558,6.5540371601,-2.4690976243 C,0.554473601,6.2390288274,-1.7716954442 C,1.3860631677,5.3730180972,-1.0731685738 H,2.4447693508,5.6156812992,-1.005430891 C,-4.9089712303,-3.6804852654,-1.5020509318 H,-5.2172104605,-4.6641098091,-1.8414543485 Al,2.0364195787,2.7325785098,0.1216098663 C,0.7658286444,1.285486808,0.0567682333 C,5.0366653152,-3.5625961532,-1.1559022857 C,3.4033955408,-1.4086431009,-0.3813096419 C,2.8982024142,-2.7258327422,-0.2635067978 C,3.7535233698,-3.7752863087,-0.6721617927 H,3.3951776105,-4.8001641474,-0.5978062977 C,4.702515643,-1.1966399928,-0.8736685361 H,5.0881352011,-0.1801127194,-0.9323681629 C,5.5126396068,-2.2534426562,-1.2549583287 H,6.5125221463,-2.0557890892,-1.6287666724 N,2.7365533443,-0.1457265681,-0.0067033787 C,0.4545453363,-1.1469946849,0.0278439048 C,-0.3731496111,-3.5818655003,1.4597276364</p>

	<p>C,4.1962841622,-0.2567795455,1.9976325949 H,4.2352020544,-1.3348768836,1.8833373401 C,3.4577656779,0.5348177539,1.1127303938 C,1.2599073114,-0.020363539,0.0596374069 C,-0.351922584,-4.2946078602,2.6634244527 H,0.5840367577,-4.7305143743,3.0030135669 C,3.3831377129,1.934078645,1.2766858977 C,-1.6124416565,-3.0466620285,1.06242005 C,-2.7587620302,-3.1701099318,1.8457605862 H,-3.7072195652,-2.7389163878,1.5505800094 C,-1.4896145674,-4.4521422695,3.4527178328 Al,1.0292414526,-2.981304345,0.2461427884 C,4.8968604635,0.3391456177,3.0429886819 H,5.4634526097,-0.2858904702,3.726392299 C,4.8682287043,1.7204143997,3.2094226763 C,4.1086561001,2.4953407732,2.3365080088 H,4.0735365229,3.5712160373,2.4907355485 C,-2.6870583937,-3.8759011553,3.0461694292 H,-3.5803837576,-3.9710726057,3.6550688697 C,-4.7928446319,2.9104511482,1.1087134961 H,-5.7264107645,2.3622934412,0.999414294 H,-1.4953253537,4.850036102,1.5753291535 H,-3.5641867375,5.6898347467,2.5980465879 O,-1.2553299476,-2.2237382573,-2.5508882219 C,-0.9442449277,-2.7400282922,-1.5049512212 O,0.0254037442,-3.5346652424,-1.2852648037 O,3.04983915,2.0253282657,-1.5657125125 C,2.8059103444,0.8864000677,-1.8437069916 O,2.5450522607,0.0466994897,-2.6317061219 H,5.661055402,-4.4001492555,-1.451089878 H,-1.4379848537,-5.0090498201,4.3831949175 H,-6.858376044,-2.7866667252,-1.7329470603 H,-5.7165976983,4.4693193767,2.2709813418 H,0.9517706478,7.1418214403,-2.2250136269 H,5.4207503379,2.187079127,4.019144186 Na,1.1665136613,-1.8045140796,-2.7460041942</p>
	<p>1CO₂-B₃P₃-NG-Na/CO₂ E=-3252.07368137H; FreqIm=1 C,-0.3093011898,-5.3306293446,2.6736375575 C,-1.3063493099,-3.5132192242,0.8208596579 C,0.096835249,-3.718509853,0.8729772555 C,-2.1838811714,-4.224955236,1.6379572162 C,-1.6829394392,-5.1372001008,2.5652325829 P,3.3756369951,-0.7275701931,-0.9578849129 P,-1.8888819197,-2.2807317813,-0.3784462735 C,0.7050908912,-1.3857945715,-0.2941248473 C,2.5645033055,-3.3648496096,-0.2822900936 C,1.6789403475,-0.3834586467,-0.4486857048 C,-4.6195203559,-2.4364522805,-0.0817322157 H,-4.4608598053,-3.5046536248,-0.2141969832 C,-3.5210542907,-1.5617406563,-0.0183600422 C,-0.6539408307,-0.9824119928,-0.1912668882 C,2.8369184923,-4.7491834411,-0.3180539792 H,2.0221033821,-5.4488880249,-0.1559214781 C,-3.7173981522,-0.1642663675,0.0641962326 C,3.637927583,-2.4876530633,-0.5918071513 C,4.9098809634,-3.0001940037,-0.8841530991 H,5.7125987039,-2.3279150544,-1.1798065811 C,4.1035097995,-5.2507302654,-0.5871049862 B,1.1260681316,-2.8604001861,0.0349813849 C,-5.9207930032,-1.9506980624,-0.0191793898 H,-6.758878759,-2.6396802743,-0.0579056205 C,-6.1391681661,-0.5749459441,0.0658829386</p>

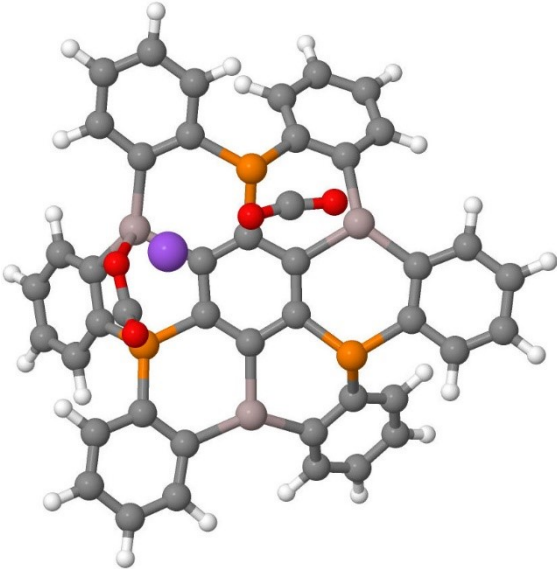
	<p> C,-5.0497119475,0.2932073908,0.0978767636 H,-5.2274199977,1.3660477488,0.1654317844 C,5.1519465873,-4.3687345281,-0.8490510918 H,6.1464265079,-4.7474166789,-1.0655852826 B,-2.5383217599,0.9275986209,0.082319311 C,-1.046276518,0.3476092454,-0.1312605031 C,2.7035633853,5.886277115,-1.1171404438 C,0.6858668481,4.1184875481,-0.4617198108 C,2.0192961675,3.6294485432,-0.4598134523 C,3.0104365064,4.560884563,-0.8055602929 H,4.0452380614,4.2338487551,-0.8535033711 C,0.3644683217,5.4440450803,-0.7604387273 H,-0.6711037519,5.7755629268,-0.763337302 C,1.3855413994,6.3345717153,-1.0849993601 H,1.1484000255,7.3654819958,-1.3269304052 P,-0.6262382522,2.9589857136,-0.1433166333 C,1.3438269625,0.9942674077,-0.3662746925 C,3.7901637943,1.6836795029,0.3900942357 C,-1.5267677106,3.9821460257,2.3468744816 H,-0.8062291703,4.7935556958,2.2798062791 C,-1.6372746898,3.0318417398,1.3353640262 C,-0.0057423292,1.2846106975,-0.2085468943 C,4.5246229812,2.5465304432,1.2260306199 H,4.163129317,3.5579305159,1.3942185148 C,-2.5459933314,1.952702862,1.3540955763 C,4.2638040792,0.3503782022,0.238872586 C,5.4355696206,-0.058462126,0.8733279107 H,5.7943879417,-1.0776196769,0.7636315921 C,5.6814306534,2.1297266547,1.8767233917 B,2.4138381134,2.1212486402,-0.188470876 C,-2.3602676815,3.8540657685,3.4566434513 H,-2.3005865361,4.5746321087,4.2659145843 C,-3.2615796643,2.792101748,3.5246541155 C,-3.3525012202,1.855789433,2.4904307037 H,-4.0630202484,1.0370582085,2.5754008774 C,6.1349652846,0.8251610219,1.6960166274 H,7.0307781997,0.4843464321,2.2070137171 C,0.5588321262,-4.6301021044,1.8389269582 H,1.6281199927,-4.7741853862,1.9606406504 H,-3.2539965579,-4.0482389559,1.5923664174 H,-2.3667140798,-5.6754620344,3.2145416395 O,-2.7821549907,1.8542709355,-1.2145612108 C,-1.9616670122,2.8492303428,-1.4794005318 O,-2.009785231,3.5857853678,-2.4264059772 O,-1.0325193068,-3.3202084528,-2.9793525107 C,-1.7914595083,-2.4626127625,-2.7029109481 O,-2.5300570458,-1.5635740846,-3.030384433 H,3.5002854149,6.5714689753,-1.390312217 H,6.2216946878,2.8131160884,2.5241200548 H,4.2718337515,-6.3229116225,-0.6104877121 H,0.0880015143,-6.0210447609,3.4111943064 H,-7.1515162074,-0.1834350985,0.1032786107 H,-3.9025381934,2.6909969083,4.3956045996 Na,-3.6817357542,0.2757853863,-2.5962532864 </p>
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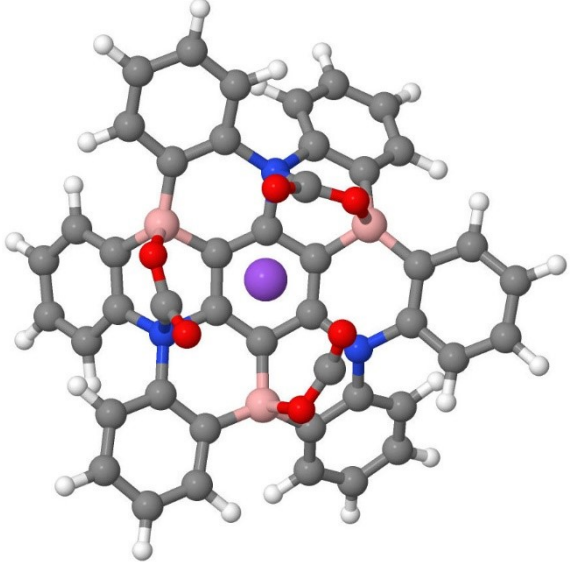


1CO₂-B₃P₃-NG-Na/CO₂ (2)

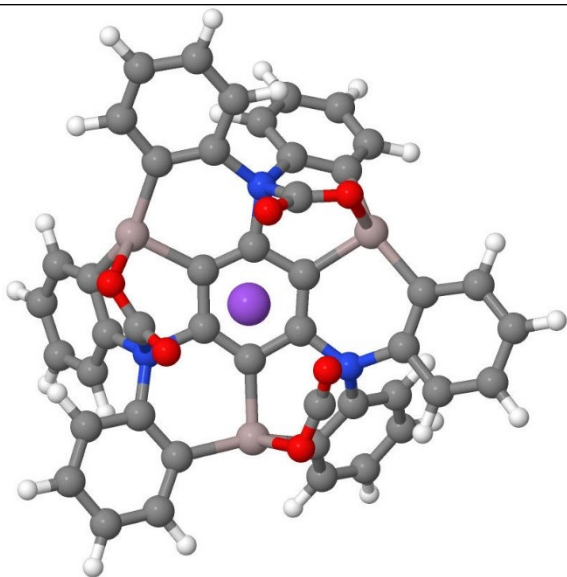
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 C,1.0051712672,-1.1113397152,-0.0633530982
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 H,-3.2947311689,-4.5747527956,-0.105082435
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	<p>1CO₂-Al₃P₃-NG-Na/CO₂ E=-3904.71481587H; FreqIm=1 C,-5.4289238203,-0.6927181269,3.2566210714 C,-3.9188134034,0.3728650998,1.2088971034 C,-3.8122082548,-1.017776887,1.4509577817 C,-4.7413441204,1.2196499675,1.9599130738 C,-5.5016359985,0.6733767311,2.9909276836 P,0.8256168615,-2.9564724387,-0.2800244924 P,-2.8901902807,1.0519691584,-0.1180483434 C,-0.9272973391,-0.7739730924,0.2030417341 C,-1.9333059495,-3.8159017367,0.1537922054 C,0.3967777483,-1.1942950632,0.0846946263 C,-4.6162009493,2.9785634498,-0.9288030178 H,-5.3051302362,2.1433125514,-1.040661493 C,-3.2952684484,2.7664717685,-0.5130512763 C,-1.1256441765,0.6225054254,0.0949292664 C,-2.8493030124,-4.8850971191,0.1879815808 H,-3.9049464669,-4.6754478229,0.3563921851 C,-2.3761107932,3.8332335029,-0.3617195479 C,-0.5703540681,-4.1356955278,-0.0632271492 C,-0.1873455322,-5.4714968621,-0.2868995064 H,0.8525384904,-5.7127740222,-0.500719472 C,-2.4612045706,-6.2097548447,0.0124235411 Al,-2.5045197124,-1.960197177,0.2975925394 C,-5.0554338281,4.271297419,-1.1983819076 H,-6.0764602618,4.4368981058,-1.5270839912 C,-4.1805014299,5.3443928157,-1.0422044013 C,-2.8659497156,5.1211750829,-0.6330191939 H,-2.2022948742,5.977745806,-0.5334692871 C,-1.1198464813,-6.5008482623,-0.2341434914 H,-0.799817701,-7.526241497,-0.3937973259 Al,-0.4830763344,3.4785678733,-0.0023040732 C,-0.127417607,1.5716018084,-0.0970711476 C,6.8964463808,1.2060010118,-0.8862794242 C,4.1519069708,1.7854112298,-0.6769525959 C,4.5996727211,0.457745358,-0.4743365164 C,5.9801768534,0.2038020196,-0.5865474833 H,6.35037668,-0.8100617949,-0.4417450319 C,5.0788447641,2.7852686955,-1.0201575528 H,4.7352022272,3.7988543561,-1.2209508871 C,6.4376048044,2.5044484341,-1.1073144683 H,7.1356421571,3.296944153,-1.3607695414 P,2.4079202593,2.3866323057,-0.7305169971 C,1.483466136,-0.2873082179,-0.0928109928 C,3.3839103302,-2.6726141375,0.7865673464</p>

	<p>C,3.3753662329,4.0437246135,1.4046905571 H,4.3132958064,3.5005038924,1.3373367737 C,2.2839757528,3.6737374227,0.6176163482 C,1.207355077,1.0819847925,-0.1647073986 C,4.4557044917,-3.0673407282,1.6008594537 H,5.3936752524,-2.5159873441,1.5622950636 C,1.0569817611,4.3828460835,0.7367526852 C,2.1753137283,-3.4090731939,0.8910336332 C,2.0643505862,-4.4799655916,1.780931677 H,1.1308741345,-5.0262628962,1.8789376994 C,4.3569448814,-4.1524036817,2.4728015739 Al,3.3206520138,-0.9428531993,-0.1093702646 C,3.2747581358,5.1161164921,2.2953094721 H,4.134415179,5.388320804,2.901007185 C,2.0867378458,5.8291285628,2.4115034695 C,0.9836037704,5.4467087795,1.6467577886 H,0.0513142886,5.9967187728,1.7651138489 C,3.1558532943,-4.8479856684,2.568919731 H,3.059020186,-5.6777608492,3.2629864357 C,-4.5943220831,-1.517640487,2.4994682629 H,-4.5535172267,-2.5778654147,2.739648546 H,-4.7906054935,2.2858139388,1.7543817701 H,-6.1450721035,1.3148242507,3.5847639562 O,0.4749232091,-2.0038893993,-3.2042215732 C,1.5365695522,-2.0189440381,-2.688078695 O,2.6791521986,-1.8534214344,-2.4833151433 O,-3.1622370252,-1.3241521953,-1.3969524379 C,-3.1398067369,-0.0502300909,-1.6408729733 O,-3.0604819625,0.4298507068,-2.7601784964 H,7.9553294919,0.9780234143,-0.9627057009 H,5.2076675688,-4.4436969196,3.0815980363 H,-3.1965018221,-7.0079167802,0.0530912251 H,-6.023057683,-1.1167512074,4.0610046475 H,-4.5208102728,6.3551078336,-1.2467048072 H,2.0146733273,6.6684718939,3.0964699044 Na,-1.8048803752,-1.5552666335,-3.2908903843</p>
	<p>2CO₂-B₃N₃-NG-Na/CO₂ E=-2580.79374829H; FreqIm=1 C,-5.4421888587,1.0842272066,2.5271915517 C,-3.2635888368,1.6328963873,0.8943043787 C,-3.7408360421,0.3094069026,0.9759834148 C,-3.8335897959,2.6613810499,1.6370141416 C,-4.929902739,2.3762623037,2.4516067557 N,-0.5553355647,-2.7055883201,-0.0432217991 N,-2.0715199819,1.8598241452,0.0350227187 C,-1.3565506518,-0.3885515914,0.4377889505 C,-3.066539438,-2.2643923446,-0.1164925683 C,-0.3307214337,-1.2923653584,0.4192895851 C,-2.7930108704,4.0196248365,-0.7976267873 H,-3.7824004319,3.5798794187,-0.8949705878 C,-1.7340994251,3.2567467457,-0.2950241722 C,-0.9866023301,0.9664137343,0.4305311217 C,-4.3340394461,-2.7947867572,-0.4091811552 H,-5.1993768777,-2.1441423598,-0.3092234901 C,-0.4286011813,3.7759525975,-0.2303642055 C,-1.9727095448,-3.127287195,-0.281273975 C,-2.118396804,-4.423776968,-0.7709866398 H,-1.2469294066,-5.0547930734,-0.9261969637 C,-4.5053701257,-4.0978306946,-0.8584212598 C,-2.5865930391,5.3417774284,-1.1653908614 H,-3.4170529831,5.9273097183,-1.5470016269 C,-1.3146590406,5.9054339022,-1.0513744961 C,-0.2604317146,5.1189393492,-0.6060917986</p>

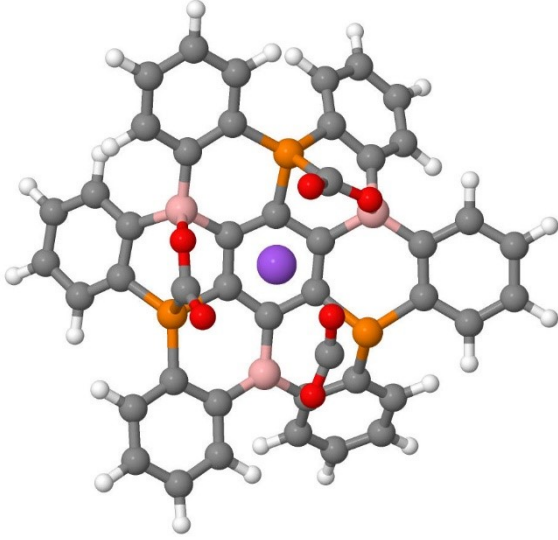
	<p> H,0.7423091001,5.5397701671,-0.571323268 C,-3.3881436168,-4.911299669,-1.0522848989 H,-3.5014359364,-5.9228625433,-1.4286277179 C,0.3181568182,1.3832182471,0.4151344643 C,5.8128896605,-1.8155160664,-0.8883654517 C,3.7045505083,-0.1228253403,-0.2734245058 C,3.4783629643,-1.5058543732,-0.2178756201 C,4.5749674955,-2.3289787163,-0.522399153 H,4.4307607216,-3.4068072223,-0.4953777456 C,4.9242284614,0.4136829936,-0.6861969225 H,5.0512985287,1.4897287939,-0.771131257 C,5.9822549461,-0.4339684429,-0.9851921044 H,6.9325343848,-0.0143256686,-1.2991254839 N,2.6302866242,0.8956757051,-0.0254886672 C,1.0242623927,-0.9581223037,0.4128130781 C,1.6225130214,-3.368954262,0.9101420839 C,4.114248606,1.9364089187,1.7501517833 H,4.7738245065,1.0771764264,1.7384978873 C,3.0087925415,2.030257035,0.9164462048 C,1.2889477588,0.3805225921,0.4099046381 C,2.3888820283,-4.1450201713,1.7778591978 H,3.458293679,-3.9631474275,1.8489038096 C,2.0981997468,3.09514649,0.9638389183 C,0.2461762759,-3.627882174,0.8642354167 C,-0.379873463,-4.5697612652,1.6682992524 H,-1.4529268691,-4.7179499075,1.6551058694 C,1.7970403689,-5.1280337532,2.5724708687 C,4.3548977677,2.9904150591,2.6339644586 H,5.2155308714,2.9397164513,3.2930207803 C,3.4985766641,4.0870706879,2.6795875309 C,2.3712577781,4.1290706549,1.8577590581 H,1.6806345446,4.9658895032,1.9261762888 C,0.420400617,-5.3289390855,2.5246557201 H,-0.046867981,-6.073248128,3.1611931526 C,-4.8398055438,0.0593538836,1.7993314201 H,-5.2134602904,-0.9574539821,1.8909925965 H,-3.4327261879,3.6676289092,1.6059816987 H,-5.3732010718,3.1749691794,3.0378167443 O,-0.5828649471,-2.222343599,-2.3966376803 C,0.151837709,-2.5104052097,-1.4827355142 O,1.4120962994,-2.5315374418,-1.4259144712 O,1.5316788224,2.5433242854,-1.3937532015 C,2.1422708499,1.4485859191,-1.4663559313 O,2.2984556018,0.687472255,-2.3931463 O,-3.0670899614,0.0640975608,-1.4860804206 C,-2.2653704245,0.9604768296,-1.6500575482 O,-1.4635704643,1.4093045674,-2.4099533128 H,6.6363799988,-2.483618761,-1.1205053238 H,2.4070779079,-5.7241260188,3.2440540053 H,-5.498821602,-4.4746327821,-1.0801033351 H,-6.2940549079,0.8728955826,3.1658010872 H,-1.1475079643,6.9397642998,-1.3352643502 H,3.6976284319,4.8996750724,3.3714226881 B,-2.8617411308,-0.7405663275,0.2040988625 B,2.0328221466,-2.1123786108,0.019705758 B,0.8180398289,2.8398173587,0.0475652128 Na,0.2766039471,-0.1128052387,-3.2240005819 </p>
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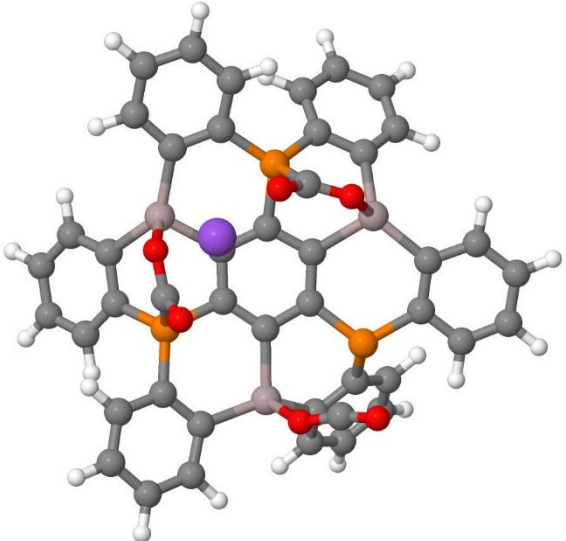


2CO₂-Al₃N₃-NG-Na/CO₂

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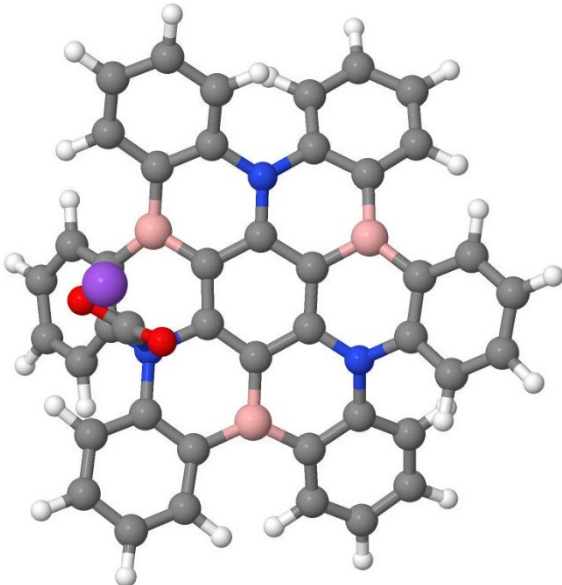
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 N,-2.7015550899,-0.935701282,-0.1312639025
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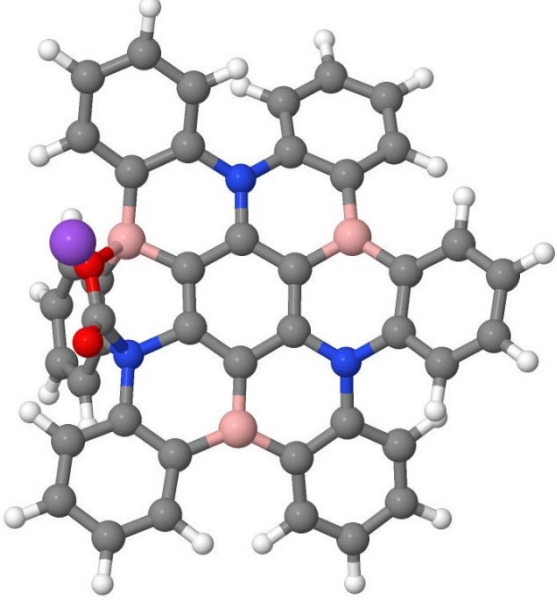
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	<p>2CO₂-B₃P₃-NG-Na/CO₂ E=-3440.59556338H; FreqIm=1 C,-4.0332496564,4.3967457623,-2.3577013411 C,-3.4585849124,2.1830218335,-0.7584169764 C,-2.4323462758,3.1338978938,-1.0116044014 C,-4.7418474031,2.3581312325,-1.2718781183 C,-5.0257055749,3.4629844255,-2.0756037388 P,2.1057493151,2.2020532721,-0.0804550509 P,-2.9816703435,0.787287525,0.3094890515 C,-0.4877640885,1.3787885787,-0.5558752857 C,0.0366598738,4.0299762109,-0.1148658501 C,0.8600538271,1.028779035,-0.5957656925 C,-5.4159293068,-0.4478101892,0.6516340085 H,-5.8008811213,0.5597686435,0.7898161031 C,-4.0682427172,-0.6557769837,0.3183708243 C,-1.4120071572,0.3110963448,-0.4345197433 C,-0.4543540539,5.309189197,0.1869479898 H,-1.5217653734,5.4921414469,0.1123999622 C,-3.5199788722,-1.9555011515,0.2322188075 C,1.429250354,3.8408240517,0.0864261487 C,2.2749829963,4.8632367851,0.5221544057 H,3.3346704935,4.6763013787,0.6823233988 C,0.3791147857,6.3410387164,0.6184287476 B,-0.9632338367,2.8819928774,-0.5325326594 C,-6.2641553896,-1.5300153543,0.8485045643 H,-7.3087577613,-1.3639111725,1.0927298512 C,-5.7516231536,-2.8237603555,0.7657360874 C,-4.4041567774,-3.0186955237,0.4777040582 H,-4.0147036405,-4.0341910055,0.4607779158 C,1.7460086478,6.1267096472,0.7745407065 H,2.3947251232,6.9282962391,1.1127046218 B,-1.9649485265,-2.2863145518,0.0000119981 C,-1.0168119033,-1.0215312618,-0.4194800356 C,5.2134795614,-3.5564195021,0.7253762739 C,2.5402767232,-3.159649125,0.1641214578 C,3.3861578238,-2.0272088053,0.1488137452 C,4.7326445245,-2.2773073576,0.4550610499 H,5.4232200148,-1.438221843,0.4950537175 C,3.0044821421,-4.453295961,0.4445826039 H,2.3150676413,-5.2945153058,0.4714056557 C,4.3521224195,-4.6537101815,0.7114324506 H,4.7232545343,-5.6508540611,0.924705882</p>

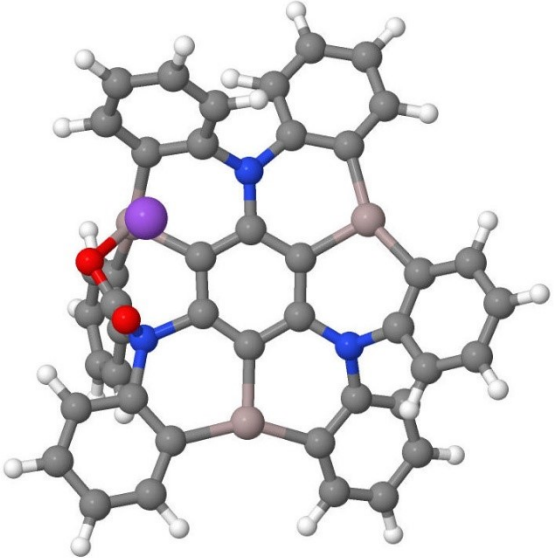
	<p>P,0.7828228402,-2.9313925237,-0.009525532 C,1.3530666449,-0.2873229692,-0.5358790561 C,3.8712154446,0.4588324537,-0.9866304023 C,0.1989818494,-5.0550967966,-1.7856538432 H,1.2465704731,-5.3446192137,-1.7907091232 C,-0.2565189681,-4.0038192039,-0.9901425826 C,0.3703178535,-1.262025268,-0.5161127387 C,4.9332372709,0.0464478867,-1.7975275181 H,5.184793655,-1.0092231775,-1.8542859409 C,-1.5970285948,-3.5569540906,-0.9572773503 C,3.5879210959,1.8439214593,-1.0108533293 C,4.3095900862,2.7779186252,-1.7531792482 H,4.038714103,3.8307132783,-1.7482226453 C,5.6755119194,0.9610347158,-2.5482017512 B,2.9083490965,-0.5034904124,-0.0902322539 C,-0.7211731249,-5.7114387401,-2.5979322384 H,-0.3995959216,-6.5353619858,-3.2267813565 C,-2.0503056942,-5.2881944485,-2.6138463253 C,-2.4777173804,-4.227383253,-1.8129447447 H,-3.5162151456,-3.9117300252,-1.8633493296 C,5.3767986123,2.3230551076,-2.522889396 H,5.9599257437,3.0241307541,-3.1111058141 C,-2.7556540419,4.2305975431,-1.826360422 H,-1.984492898,4.9551101479,-2.0768245086 H,-5.5168657915,1.6208752095,-1.0884573783 H,-6.0213595554,3.5808992415,-2.4923573654 O,1.8864497046,1.7108062916,2.6130142557 C,2.3491155495,1.2960326442,1.5672239211 O,2.8708233762,0.126345432,1.3858875419 O,-1.3963879789,-2.6447781025,1.4632660252 C,-0.1308534421,-2.7079641077,1.6367847618 O,0.4982161181,-2.4852912305,2.6610176555 O,-1.778973621,2.698807229,2.0965117991 C,-1.7645571888,1.5141380959,2.1808176448 O,-1.3238739366,0.5127102702,2.6792722641 H,6.2649589667,-3.69888715,0.9570184575 H,6.4958111166,0.6052158301,-3.1646654036 H,-0.0445443274,7.3144870606,0.8455331354 H,-4.2504929316,5.2489992539,-2.9939408691 H,-6.3973868796,-3.6776977192,0.9478052282 H,-2.762592332,-5.7881462686,-3.263766295 Na,0.7285652785,-0.3068622482,3.3261538776</p>
	<p>2CO₂-Al₃P₃-NG-Na/CO₂ E=-4093.29732378H; FreqIm=1 C,5.92616,0.049413,2.916704 C,4.028706,-0.815465,1.100246 C,4.18917,0.580944,1.280635 C,4.77594,-1.759687,1.813046 C,5.730966,-1.31636,2.724927 P,-0.229545,3.112768,-0.034737 P,2.749382,-1.377722,-0.06183 C,1.158685,0.734798,0.467767 C,2.584582,3.585734,0.004324 C,-0.0896,1.343187,0.402064 C,4.118413,-3.568072,-0.855465 H,4.931348,-2.856007,-0.986586 C,2.852917,-3.141896,-0.420947 C,1.118204,-0.675329,0.351343 C,3.641009,4.499821,-0.150879 H,4.666193,4.155486,-0.025919 C,1.768386,-4.03537,-0.25782 C,1.279671,4.105071,-0.16561 C,1.056192,5.447532,-0.511774</p>

	H,0.04585,5.821982,-0.662807
	C,3.430125,5.84024,-0.469738
	Al,2.899671,1.663428,0.252803
	C,4.340268,-4.914594,-1.116133
	H,5.316055,-5.246886,-1.455711
	C,3.302619,-5.828234,-0.935611
	C,2.046823,-5.387392,-0.521984
	H,1.253278,-6.124809,-0.414792
	C,2.133513,6.313464,-0.662764
	H,1.958623,7.351185,-0.928624
	Al,-0.081119,-3.406242,0.024539
	C,-0.03771,-1.437862,0.20336
	C,-6.848474,0.108216,-0.809288
	C,-4.29509,-0.923091,-0.328439
	C,-4.441181,0.477326,-0.492294
	C,-5.74378,0.952814,-0.726546
	H,-5.904944,2.02239,-0.854977
	C,-5.401488,-1.780838,-0.44375
	H,-5.271619,-2.858538,-0.362879
	C,-6.673747,-1.266888,-0.67026
	H,-7.521474,-1.94076,-0.748579
	P,-2.698783,-1.796035,-0.191865
	C,-1.327863,0.672042,0.259221
	C,-2.842037,3.369673,0.781642
	C,-3.761055,-3.185371,2.057271
	H,-4.60485,-2.500891,2.027606
	C,-2.70512,-3.053152,1.154224
	C,-1.263187,-0.720148,0.210837
	C,-3.848272,3.985147,1.537936
	H,-4.862674,3.594198,1.496105
	C,-1.582427,-3.923671,1.189496
	C,-1.548488,3.930535,0.898504
	C,-1.261072,5.017965,1.732271
	H,-0.250967,5.407482,1.825168
	C,-3.588559,5.084689,2.357262
	Al,-2.935204,1.710145,-0.299716
	C,-3.726388,-4.199451,3.015552
	H,-4.546734,-4.301588,3.719832
	C,-2.642108,-5.070057,3.071274
	C,-1.581407,-4.918915,2.175249
	H,-0.736585,-5.601374,2.251506
	C,-2.295897,5.596432,2.461522
	H,-2.090262,6.440378,3.1125
	C,5.160091,0.977048,2.208042
	H,5.325512,2.036399,2.392017
	H,4.617903,-2.825223,1.671477
	H,6.316438,-2.038832,3.284741
	O,0.007058,2.659235,-2.675606
	C,-0.85002,2.706192,-1.796
	O,-2.071176,2.361762,-1.874468
	O,-0.807471,-3.656877,-1.776519
	C,-1.854523,-3.260569,-2.252908
	O,-2.648916,-3.184755,-3.095165
	O,3.178966,0.912124,-1.467505
	C,2.941785,-0.354774,-1.654906
	O,2.652967,-0.834851,-2.73555
	H,-7.837501,0.517542,-0.99279
	H,-4.394737,5.538935,2.926201
	H,4.275435,6.513471,-0.578208
	H,6.67289,0.393122,3.626623
	H,3.470522,-6.883437,-1.130336
	H,-2.618162,-5.861456,3.814734
	Na,1.750121,1.407916,-3.289099

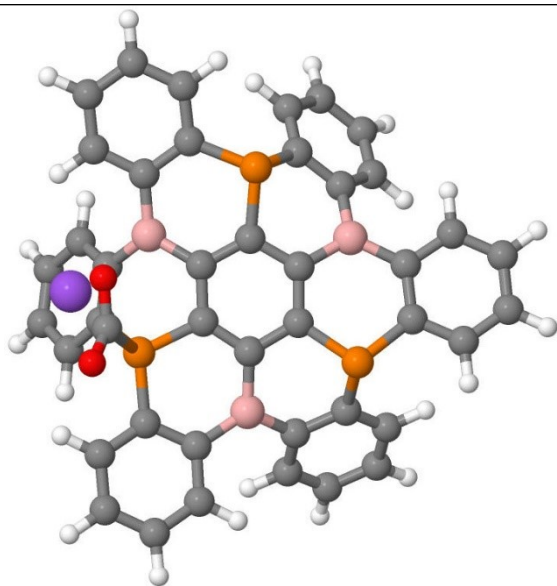
Table S8: Geometries, energies (in Hartree) and Cartesian coordinates (in Å) of the adducts with a Na⁺ cation in vacuum. Level of theory: M06-2X/6-311++G*//M06-2X/6-31+G*

	<p>B₃N₃-NG-Na inter E=-2203.83090491H; FreqIm=0</p> <p>C,0.7028823498,5.8978358965,1.7828489158 C,1.5199225153,3.5013169006,0.563000796 C,0.1415707564,3.8233145721,0.6143654557 C,2.462439076,4.358358288,1.1534556552 C,2.0553698035,5.5429029833,1.7463923915 N,-2.5244309278,0.2981153087,-0.0216252499 N,1.9716542202,2.2709895552,-0.0027010268 C,-0.2596295714,1.3548453113,0.0988092536 C,-2.388295545,2.8283780005,-0.100224179 C,-1.0335427655,0.2146698363,0.1086743725 C,3.820897694,3.3061060793,-1.211692475 H,3.259214912,4.232558428,-1.2572262508 C,3.2739999671,2.1761238226,-0.5811852278 C,1.1514258814,1.1563974451,0.036648435 C,-3.0613003116,4.028136693,-0.4000123399 H,-2.5031905632,4.9587200602,-0.3752648443 C,3.969175417,0.9460652424,-0.5993172758 C,-3.1326981231,1.6499061171,-0.2124908757 C,-4.4733268232,1.648127703,-0.5984151544 H,-5.0209491922,0.7124067312,-0.679373199 C,-4.3987944779,4.0523261441,-0.7710879393 B,-0.8616923461,2.7435952828,0.18718383 C,5.0688167955,3.2333364804,-1.8091994234 H,5.4709849306,4.1132437708,-2.3023791211 C,5.7932036221,2.0361617341,-1.8076919583 C,5.2336258353,0.9137307562,-1.2220798075 H,5.7618954874,-0.0341098373,-1.2765689885 C,-5.1083914546,2.854522258,-0.8661977414 H,-6.1533711286,2.855391998,-1.1599391948 B,3.2193161908,-0.3109217072,-0.1223355669 C,1.7185177969,-0.1311727257,-0.0151146244 C,-1.0378571999,-5.9068987821,-0.7217105697 C,0.5595188003,-3.6532473751,-0.1821891146 C,-0.8258985475,-3.6217504096,0.1101759705 C,-1.595489746,-4.772457291,-0.1560170116 H,-2.6609724644,-4.7422738347,0.0613810341 C,1.11163451,-4.7859297014,-0.8022284665 H,2.1576058035,-4.7931681965,-1.0888584716 C,0.3203239368,-5.8948581474,-1.0625973054 H,0.7665250783,-6.7584173536,-1.5470430324 N,1.3952083155,-2.5317209515,0.0981641377 C,-0.541452661,-1.0895337817,0.1401220425 C,-2.7577904344,-1.8557489726,1.1880844915 C,3.1305725259,-3.9289038908,1.1084596905 H,2.3868618815,-4.6853783627,1.3303398267 C,2.7636422879,-2.732914064,0.4705929211 C,0.861518509,-1.2525162576,0.0675340539 C,-3.3868711293,-2.6438581515,2.1536437215 H,-3.057416316,-3.6709203623,2.2894065721 C,3.7202068539,-1.7090342671,0.2850804738 C,-3.1862272051,-0.5222015279,1.0568698421 C,-4.1568625668,0.0231913882,1.8808284161 H,-4.4513572418,1.0625184912,1.8095347103 C,-4.3917420675,-2.1262317024,2.9733321034 B,-1.439923,-2.2663629013,0.4687954052 C,4.4450326365,-4.1381874351,1.496924093 H,4.7052895954,-5.0652372829,1.9989563219</p>
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	<p>C,5.4191665606,-3.1595360824,1.2796718089 C,5.0435045567,-1.9595741879,0.6997569791 H,5.7775532511,-1.1651375133,0.5993179969 C,-4.756978893,-0.7929857412,2.8468956938 H,-5.5091446265,-0.3652267719,3.5020277334 C,-0.2296189815,5.0347198619,1.2354587753 H,-1.2850300489,5.2730054302,1.3277581588 H,3.5107071563,4.0830834012,1.1746764912 H,2.7993582324,6.1835019618,2.2103589699 O,-2.1252192441,0.1861648384,-2.3857746416 C,-2.7613536968,-0.3856107271,-1.5087588268 O,-3.5199909473,-1.3479491695,-1.5205933555 H,-4.8858661797,4.9949583721,-0.9996060984 H,0.3893657101,6.8187130809,2.2636053699 H,6.765569177,1.9833981028,-2.2867409185 H,6.4439350409,-3.3245654734,1.596297004 H,-1.6453927524,-6.7838990395,-0.9213178676 H,-4.8651931937,-2.7539152992,3.7216319678 Na,-2.8538812971,-1.5079510492,-3.7142357382</p>
	<p>1CO₂-B₃N₃-NG-Na E=-2203.82816876H; FreqIm=0 C,5.0742803591,3.1563148365,1.5049550061 C,3.5392922472,1.091457106,0.369906266 C,3.0406740731,2.4186896046,0.3612556717 C,4.7712008909,0.8104918737,0.9868946124 C,5.5266893339,1.8324432894,1.5376787137 C,0.7532211937,1.3960647067,-0.1809928406 C,0.804984625,3.9418669744,-0.4336566293 C,-0.6618180279,1.4504857765,-0.178269753 C,4.6616344326,-1.0808181439,-1.243775763 H,5.1312791836,-0.1088627847,-1.3499558975 C,3.3967193647,-1.1834205171,-0.6451460627 C,1.3875616381,0.139909973,-0.2338400885 C,1.4216083521,5.1226212975,-0.892878376 H,2.5062438585,5.1834727199,-0.8726304658 C,2.7471364677,-2.43886091,-0.5988927644 C,-0.6046337814,3.8611078883,-0.511461991 C,-1.3402447159,4.9094384979,-1.0857122152 H,-2.413629895,4.8181258964,-1.211047014 C,0.6930953934,6.1789183297,-1.4147616153 B,1.5837862599,2.6589397611,-0.0754853553 C,5.3214196654,-2.2113962024,-1.7098740619 H,6.303372991,-2.103615143,-2.1606976954 C,4.7277670367,-3.4698753681,-1.6045129128 C,3.4463974988,-3.5606300852,-1.0709468136 H,2.9577245769,-4.532888261,-1.0105054023 C,-0.6955895278,6.0567522176,-1.522372663 H,-1.2803836793,6.8534580061,-1.9723668967 B,1.2051750457,-2.4934398791,-0.2692205321 C,0.625979056,-1.035338354,-0.3315651831 C,-5.6545110857,-2.3963307447,-0.9618051808 C,-2.9260854827,-2.2397225809,-0.5500988517 C,-3.6671860546,-1.0547040539,-0.4515404311 C,-5.0497584229,-1.1761294914,-0.6909402888 H,-5.6576738618,-0.2775191539,-0.6873701818 C,-3.5109872932,-3.4776854341,-0.803530397 H,-2.9030644653,-4.3774700973,-0.8469891967 C,-4.8826668935,-3.557952318,-1.0003799513 H,-5.3418372969,-4.5210514531,-1.1982026234 C,-1.4551730666,0.2796305542,-0.248718607 C,-3.5079692023,1.6473464762,0.3625480351 C,-1.8559873416,-3.4967553451,1.7931446025 H,-2.9218392756,-3.3167234486,1.7193245801</p>

	<p>C,-0.9596008546,-3.0634527938,0.8301672788 C,-0.7311021529,-0.9030020562,-0.343171654 C,-4.7849020672,1.7968800806,0.9503047672 H,-5.4574425756,0.9451282785,0.9603241586 C,0.425536147,-3.2342351134,0.9157093394 C,-2.6208515927,2.7560396412,0.4233109687 C,-3.0176656691,3.930714885,1.0893542528 H,-2.3193309846,4.7511597719,1.2052630744 C,-5.1857083563,2.9667845181,1.5656917531 B,-2.9570829634,0.3084234343,-0.1446360588 C,-1.3307118458,-4.1738758484,2.8982475283 H,-2.0065302799,-4.5211330437,3.6728940081 C,0.0389719076,-4.3925326307,3.0107379503 C,0.9108533066,-3.9194464077,2.0265421668 H,1.9827182032,-4.0686588593,2.1290158798 C,-4.2817699829,4.0334340913,1.6417677853 H,-4.5560633724,4.9440888273,2.1658652809 C,3.8417028211,3.4266357384,0.937713887 H,3.4520170868,4.4403414238,0.9710382011 H,5.123979987,-0.2116620427,1.063789602 H,6.4684179231,1.5904485636,2.0214163638 H,-6.7235367355,-2.446174898,-1.1430839095 H,0.4312058829,-4.9201605043,3.8747167641 H,-6.16967555,3.0466491366,2.0161204719 H,5.6665332819,3.950239559,1.9482354184 H,1.1937908346,7.0753127735,-1.7663987023 H,5.2525564235,-4.3575632879,-1.9445582683 O,-1.452121811,-2.9587713918,-2.6892975356 C,-0.8085981205,-2.867897675,-1.666959168 O,0.4309203343,-3.175018024,-1.5522863415 N,-1.2976140046,2.6802233613,-0.0918736999 N,2.7677509359,0.0223390572,-0.1655416786 N,-1.436043482,-2.2610958585,-0.3955579574 Na,0.6357759518,-3.3155452722,-3.7890248026</p>
	<p>1CO₂-Al₃N₃-NG-Na E=-2856.40356763H; FreqIm=0 C,5.2265060666,3.6631103861,1.6070807892 C,3.5607275232,1.6455716888,0.5487860451 C,3.1072007734,2.989778674,0.5690460573 C,4.8229744358,1.3380436151,1.0915769127 C,5.6429124787,2.3306744441,1.6064180962 C,0.5545714254,1.4962133604,0.0101318639 C,-0.1992331937,4.3569670389,-0.4494978017 C,-0.8382620122,1.2750568408,-0.0179256964 C,4.5006138901,0.0931226312,-1.6975616381 H,4.5022075615,1.1663014677,-1.8695520009 C,3.6545479492,-0.4340862227,-0.7048262035 C,1.4205352704,0.3870133158,-0.0374990879 C,-0.096536183,5.6381897436,-1.0265424053 H,0.8400732908,6.1840514546,-0.9332312835 C,3.6358879278,-1.8352926911,-0.4598625641 C,-1.4276995592,3.6639197949,-0.5839664881 C,-2.4735096208,4.2532150365,-1.3166661577 H,-3.4076098333,3.7136232465,-1.4413076715 C,-1.1460157655,6.2315622386,-1.7136461802 C,5.3408239856,-0.7312336851,-2.4403861639 H,5.9840173473,-0.2970230347,-3.2000838029 C,5.3541326531,-2.1073264792,-2.2039517767 C,4.5028043008,-2.6353076174,-1.2332313626 H,4.5062147053,-3.7122082623,-1.0747959654 C,-2.335635494,5.5175506914,-1.8700897404 H,-3.160781362,5.9445281199,-2.4324513901 C,0.9240531968,-0.9245788636,-0.1159236801</p>

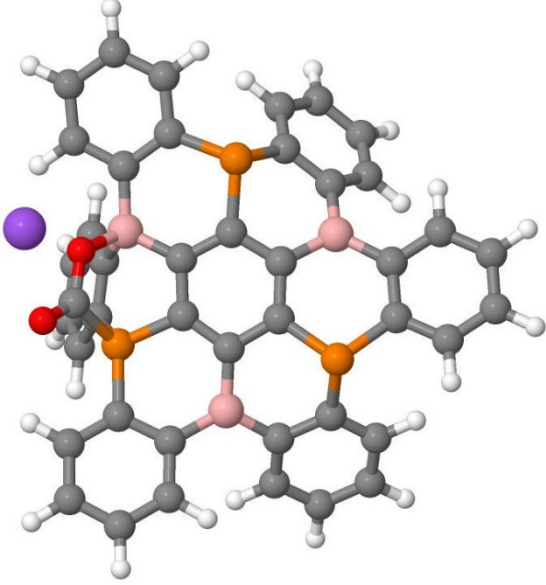
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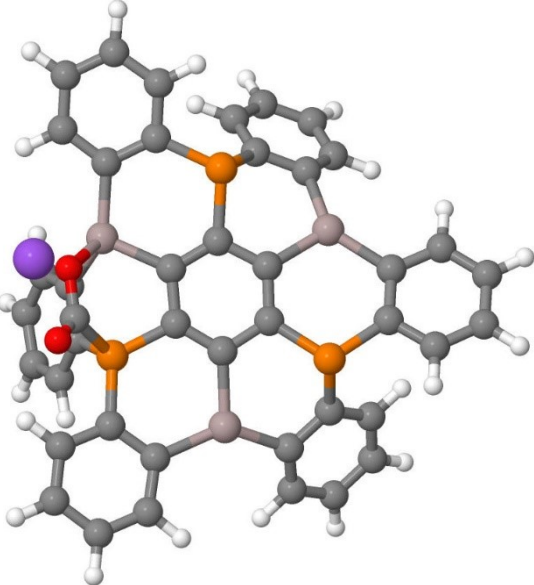


B₃P₃-NG-Na inter

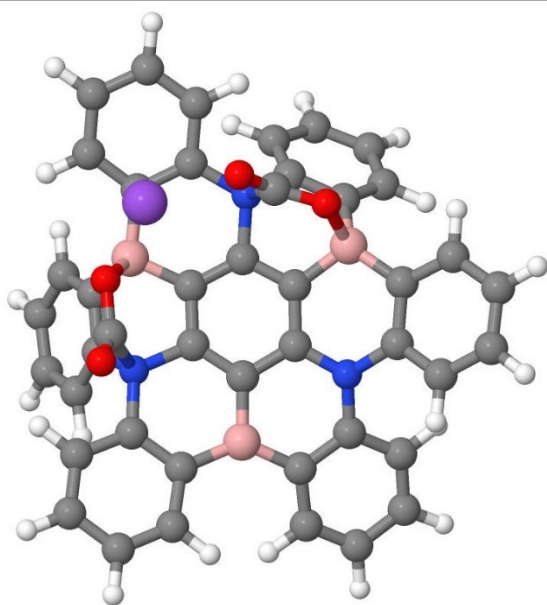
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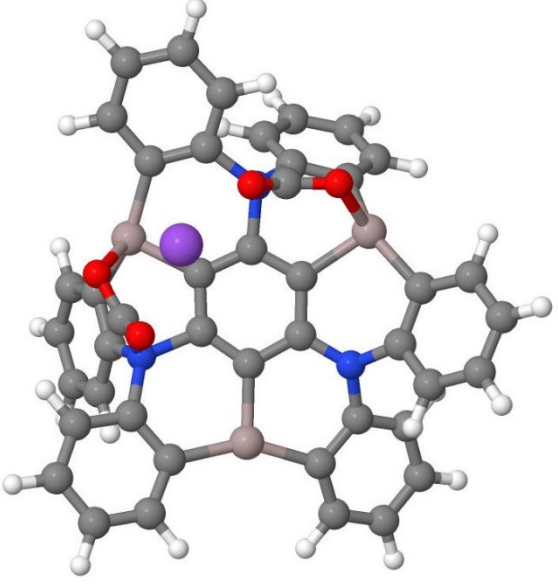
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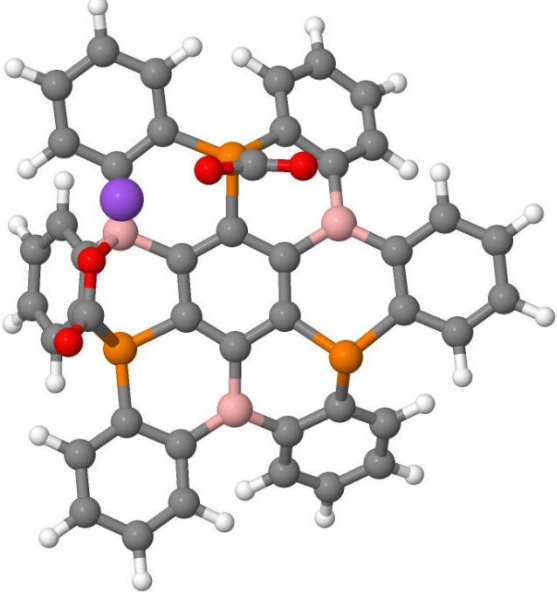


2CO₂-B₃N₃-NG-Na

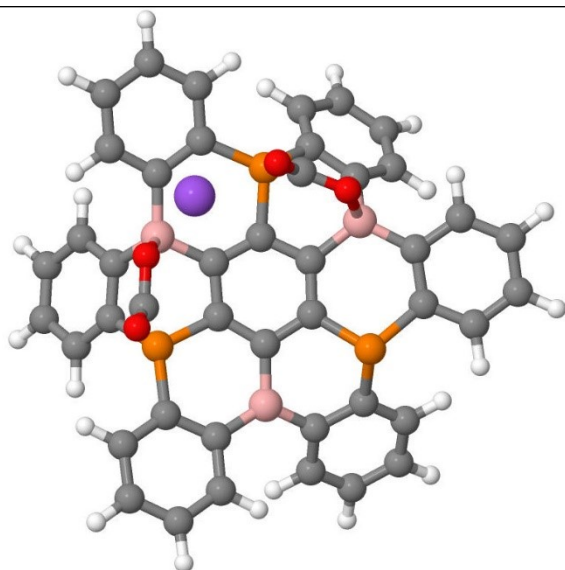
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 C,3.6334678016,1.3398730096,-0.1205736995
 C,-3.5475489866,1.1551471877,-0.2564813668
 C,-4.8742370515,1.0079368428,-0.6535523842
 H,-5.287193916,0.0208016449,-0.8395759653
 C,-5.1320109108,3.4013893185,-0.61394525
 C,4.6275377996,3.8546384605,-0.8890655987
 H,4.9846487252,4.8253618222,-1.2194973673
 C,5.4692557924,2.7440636057,-0.9240913564
 C,4.9537924034,1.5060179673,-0.562801275
 H,5.5792006684,0.6194961094,-0.650148534
 C,-5.6713829371,2.1322349188,-0.821490189
 H,-6.7041454248,2.0146346925,-1.1331259625
 C,1.4454120818,0.0495134879,0.1862543606
 C,-0.308122455,-6.0338970314,-1.1910427875
 C,0.8260672774,-3.5939247373,-0.4635141653
 C,-0.5779885296,-3.6986608965,-0.4831301807
 C,-1.1112434762,-4.9497560366,-0.8536544386
 H,-2.1943389516,-5.0577152639,-0.8718666293
 C,1.6445823389,-4.6691092503,-0.823215909
 H,2.7246034624,-4.5491141166,-0.8353997735
 C,1.0809980199,-5.8868178704,-1.1785724681
 H,1.7258272248,-6.7153383228,-1.4533282314
 N,1.5565711658,-2.3239288218,-0.1862892391
 C,-0.648439476,-1.1865476498,0.0695375731
 C,-2.7443342306,-2.3841453927,0.8157666734
 C,2.7272468533,-3.5206213247,1.7257825583
 H,2.0535395494,-4.3664371734,1.6560311333
 C,2.6318822166,-2.4221428035,0.8823018642
 C,0.7211661556,-1.1143185661,0.0907843146
 C,-3.2011211863,-3.327476693,1.7332620724
 H,-2.7518339764,-4.3176378093,1.7485770246
 C,3.4446505472,-1.2887431065,1.0013727589
 C,-3.3419054037,-1.1186269063,0.8436046625
 C,-4.32221544,-0.7565545463,1.7545542221
 H,-4.740974436,0.2421620033,1.7850900057
 C,-4.2085711187,-3.0074614485,2.645817225
 C,3.7225711131,-3.5041585437,2.7055822263
 H,3.8151710063,-4.3512776955,3.3775430944
 C,4.5785524569,-2.4128354721,2.8282809304
 C,4.4299597295,-1.3091874912,1.9871033324
 H,5.0729903056,-0.4407341877,2.1060082074
 C,-4.7552697925,-1.7277859758,2.6612727056
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	<p>H,2.6183899348,4.3380458667,1.8706516298 H,1.5512946106,6.2628312636,2.9328428009 O,-3.1856110434,-0.2050610185,-2.5416355045 C,-2.7581540315,-0.8218648814,-1.6228034314 O,-2.2144189508,-1.9952947761,-1.5997161345 O,3.0670788498,-0.9141931116,-1.4425118617 C,2.2153007841,-1.7991617289,-1.6156111185 O,1.7008925465,-2.2911682856,-2.5959024151 H,-0.7551987248,-6.9841297802,-1.4665424727 H,-4.5551434394,-3.7516602226,3.3561158184 H,-5.7414863259,4.2858403401,-0.7697977452 H,-0.9160228492,6.5968667431,2.772816545 H,6.4963136918,2.8400912274,-1.2615727874 H,5.3489689257,-2.4143819531,3.593171041 B,-1.4621557474,2.5474128656,0.3816042548 B,-1.5276347593,-2.4454759724,-0.2119616388 B,3.0030242681,-0.0917150459,0.0463954824 Na,-0.4670692441,-2.7782483092,-3.009313052</p>
	<p>2CO₂-Al₃N₃-NG-Na E=-3044.93106964H; FreqIm=0 C,4.0860353448,-4.1346257481,2.7534132393 C,1.9203867827,-3.0990645779,1.2682193983 C,3.1934330251,-2.4740415518,1.1893717513 C,1.7548212979,-4.206007106,2.1194516514 C,2.8184116918,-4.7157042693,2.8473515874 N,1.7737304221,2.1666011366,-0.1697734941 N,0.7563259027,-2.7201369867,0.5065656222 C,1.319447864,-0.3365605144,0.2684939372 C,4.0391887734,0.880385563,-0.2032424001 C,0.8369278369,0.942533788,0.101553289 C,0.8910050069,-4.8074297425,-0.6908719635 H,1.9675308744,-4.6671651243,-0.6677049853 C,0.0540263436,-3.8310409995,-0.1237376294 C,0.3508981344,-1.3773436257,0.3424153675 C,5.4139516955,0.9915150144,-0.497635753 H,6.0636656478,0.1422302916,-0.2992348007 C,-1.3537972608,-3.9932864965,-0.1924155426 C,3.2530672254,2.0062176925,-0.4819387171 C,3.7999219568,3.1727626378,-1.0192834477 H,3.1725596542,4.044897412,-1.1961083233 C,5.9752877727,2.1426490625,-1.0347031084 Al,3.1612937168,-0.7401550462,0.3906775718 C,0.3699235962,-5.9572613644,-1.2677297315 H,1.0459916143,-6.6925307345,-1.6940258342 C,-1.0087029382,-6.1577776355,-1.3058487943 C,-1.8405133255,-5.1717934137,-0.7897404337 H,-2.9165933618,-5.3196377676,-0.8567009338 C,5.1568121671,3.2400676273,-1.3012621497 H,5.5719235266,4.1507342625,-1.7208918038 Al,-2.4346424346,-2.4158159413,0.1261616141 C,-1.0112476709,-1.0898530791,0.1878089846 C,-4.9026359759,4.0444990085,-1.4130146318 C,-3.4378682532,1.7977544842,-0.6472024691 C,-2.8213649241,3.0568381976,-0.5409261377 C,-3.6035177163,4.1642065739,-0.9391140274 H,-3.1706008791,5.1600345864,-0.8722829909 C,-4.7447850713,1.6622148444,-1.1285910846 H,-5.2059470703,0.6777145184,-1.1818693273 C,-5.4746653699,2.7758809877,-1.5128258106 H,-6.4874503927,2.6515217137,-1.8824515363 N,-2.8696790045,0.4490729637,-0.2335633437 C,-0.5027236045,1.3118465836,0.018046404 C,0.4060900744,3.8396631111,1.2124852877</p>

	<p>C,-4.3120187322,0.8683236664,1.7760864164 H,-4.2622017664,1.9296415376,1.5648210608 C,-3.684503594,-0.0788262885,0.9666184964 C,-1.366613247,0.2406206954,0.0456465599 C,0.3456483972,4.7000405146,2.3144193284 H,-0.5748392483,5.243836111,2.5105544494 C,-3.7068060996,-1.4522027694,1.2604411953 C,1.623598897,3.1685253118,1.0003437534 C,2.707613641,3.3041571639,1.8662168885 H,3.6364359455,2.7682372707,1.7152477955 C,1.4233221422,4.8725826214,3.1808736539 Al,-0.9403982775,3.1948328199,-0.0402117164 C,-5.0295799309,0.4370573993,2.890189965 H,-5.5193957717,1.1730711189,3.5198255465 C,-5.1180469808,-0.9188250873,3.1863421027 C,-4.4524899368,-1.8401250679,2.3804350991 H,-4.5023184781,-2.8944727492,2.6404873352 C,2.5968639516,4.1611961869,2.9603208725 H,3.4411698511,4.2668581909,3.6339981722 C,4.2513939102,-3.0208484531,1.9449999376 H,5.232742862,-2.5534288014,1.8960089788 H,0.7767018034,-4.6715416822,2.1940700049 H,2.6557709033,-5.5689533083,3.4991548969 O,1.5001732484,1.924968022,-2.5078412146 C,1.1345035533,2.588526395,-1.5656462242 O,0.216797391,3.464339028,-1.5319536355 O,-3.2195816074,-1.6330196797,-1.4548967712 C,-2.9247109825,-0.4338120322,-1.6072774026 O,-2.5839583338,0.2031131563,-2.581823556 H,-5.4656490836,4.9260226557,-1.7034458957 H,1.34286313,5.5466813148,4.0280385498 H,7.0389455083,2.1878587188,-1.2458763276 H,4.9210850834,-4.5376216392,3.3174682764 H,-1.4255800422,-7.0570090876,-1.7485955646 H,-5.6865998569,-1.2543176143,4.048386373 Na,-0.7734419442,1.4181420249,-3.0591579004</p>
	<p>1CO₂-B₃P₃-NG-Na inter E=-3252.07621555H; FreqIm=0 C,-0.3300641811,-5.4667296579,2.5689159151 C,-1.3407242431,-3.5343210979,0.862060988 C,0.0576380859,-3.769676696,0.8458550794 C,-2.2107709879,-4.2562297318,1.6772767173 C,-1.7008167177,-5.2323546419,2.5314956001 P,3.3395436059,-0.7447777713,-0.9475683575 P,-1.9072668186,-2.2122024916,-0.2179026549 C,0.687285233,-1.3755662699,-0.1968965088 C,2.4917739475,-3.3936410504,-0.3751704742 C,1.6689098625,-0.3868258865,-0.3694746225 C,-4.639625886,-2.3822445519,-0.0113163028 H,-4.4816835579,-3.4540914737,-0.1071204178 C,-3.5453714668,-1.5057194671,0.0609606169 C,-0.6547249918,-0.9430534853,-0.0436006819 C,2.7332346575,-4.7784929229,-0.4963065388 H,1.9032447392,-5.4678575915,-0.3704901622 C,-3.7256034626,-0.1045316143,0.0973831188 C,3.5794048704,-2.5205309099,-0.6475269057 C,4.8382111774,-3.0419291737,-0.9789036542 H,5.6525073437,-2.3713677665,-1.2452112797 C,3.9861445615,-5.2892816099,-0.807314815 B,1.074759299,-2.883835617,0.0127311082 C,-5.9378186373,-1.8852721534,-0.0065553195 H,-6.7799724801,-2.5683960405,-0.0539229063 C,-6.1456902018,-0.5061077273,0.0313445364</p>

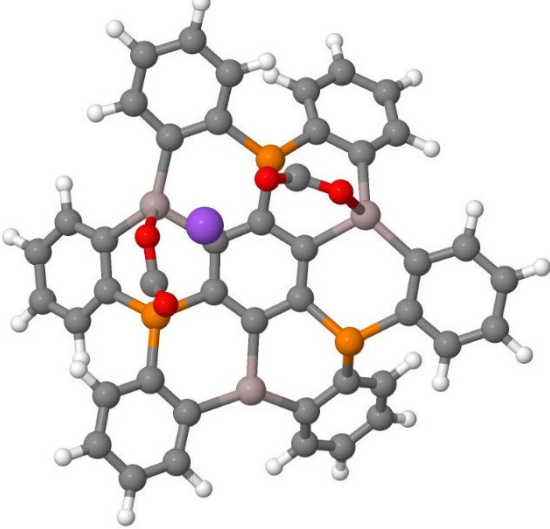
	<p> C,-5.0540851286,0.3588903105,0.0732080405 H,-5.2288342517,1.4335243456,0.0974645631 C,5.0513141343,-4.4149035285,-1.0243269073 H,6.0360215601,-4.80057859,-1.2710067226 B,-2.5379578254,0.981602807,0.1262144226 C,-1.0401768979,0.3857469025,0.0038240812 C,2.7867667589,5.8591958802,-1.0771862163 C,0.7421914593,4.1226079024,-0.4173360905 C,2.0701555137,3.6161553,-0.4044057801 C,3.0743225172,4.532164835,-0.7536141862 H,4.1046602744,4.1909596212,-0.7962198915 C,0.4405956213,5.4493664308,-0.7301966702 H,-0.5904997041,5.7947735743,-0.7420144654 C,1.4747222536,6.3244533429,-1.0562198091 H,1.2518513717,7.3560888535,-1.308380031 P,-0.5929628715,2.9881717654,-0.1006978799 C,1.3528163318,0.9939136238,-0.2644095141 C,3.8281360568,1.639755905,0.4195297239 C,-1.5894711741,4.1186600419,2.3038111299 H,-0.8550376649,4.9175194935,2.2371548566 C,-1.6673434555,3.1290905489,1.3274060674 C,0.0121251917,1.3088850211,-0.086841857 C,4.5965307131,2.480972439,1.2466874115 H,4.2559990333,3.4962096847,1.434899119 C,-2.5911999053,2.0618401411,1.3493955362 C,4.2760440074,0.2997482896,0.2425300015 C,5.4554087917,-0.1352588318,0.8437906355 H,5.7944777903,-1.1588509674,0.7137081562 C,5.761326098,2.0374196785,1.8651004162 B,2.446599649,2.1056461748,-0.1235959496 C,-2.4732233576,4.0468705273,3.3791615758 H,-2.4396455108,4.7996595277,4.160067451 C,-3.3910720771,2.9994850654,3.4498540519 C,-3.4479985733,2.0220424814,2.452078999 H,-4.1724178865,1.2159395938,2.5395767989 C,6.1886384474,0.7277958877,1.6593568834 H,7.0906592819,0.3668103769,2.1449399401 C,0.5284330604,-4.7443345257,1.7408283209 H,1.5964952947,-4.9250309282,1.8128320788 H,-3.2753794686,-4.0438564372,1.6837264647 H,-2.372356094,-5.7883495826,3.1781687614 O,-2.7049280447,1.8377824599,-1.2243472521 C,-1.8690106779,2.8201589979,-1.4916083357 O,-1.8646807302,3.5094043108,-2.4743314798 O,-0.8274010658,-3.3715188872,-2.3958518779 C,-1.6812112069,-2.5482400295,-2.1683359499 O,-2.3975941591,-1.7595318025,-2.8061925319 H,3.5938473325,6.5314137748,-1.352043557 H,6.3282653704,2.7043886616,2.5067488365 H,4.1312281352,-6.3612102647,-0.8982151619 H,0.0758269288,-6.2084582535,3.2499366021 H,-7.1559290741,-0.1075379789,0.0215209898 H,-4.0719515515,2.942352353,4.2940659374 Na,-3.3740533724,0.1722080765,-2.6962288142 </p>
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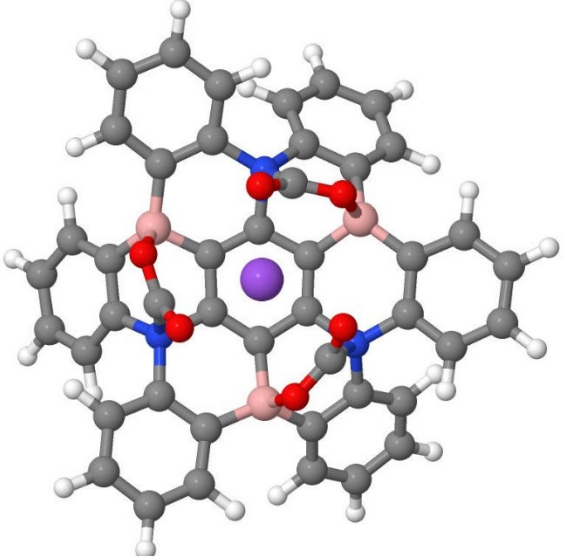


2CO₂-B₃P₃-NG-Na

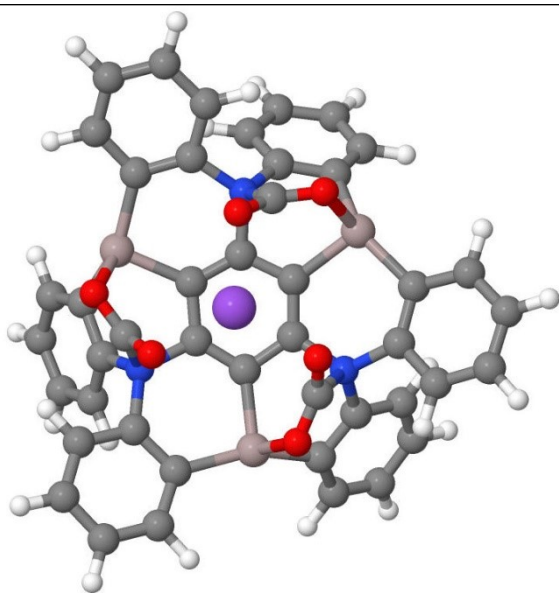
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 C,-1.5978692979,-3.4372995614,0.8868019563
 C,-3.8501416658,-2.9938509987,1.8434439357
 C,-3.696426608,-4.0712859071,2.7100155107
 P,2.6604622623,-1.8026966059,-0.484561396
 P,-2.7154796314,-1.3120358796,-0.1355075521
 C,-0.0742127254,-1.4072912405,0.0625921228
 C,0.8107181313,-3.9528397997,-0.3256969657
 C,1.2048290108,-0.8509647443,0.0204609231
 C,-5.3188662281,-0.5977612229,-0.5983886828
 H,-5.5204887052,-1.6662790455,-0.5581240445
 C,-4.024813308,-0.1107121403,-0.3576115006
 C,-1.1525149436,-0.5093451433,0.1669674139
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 H,-0.4729160166,-5.6574955278,-0.5822685686
 C,-3.7080885117,1.2696505536,-0.4204303894
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 C,2.2486982377,4.965306639,-0.6430460056
 H,1.4246639715,5.6509258197,-0.827861324
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	<p>2CO₂-Al₃P₃-NG-Na E=-3904.75700286H; FreqIm=0 C,-5.707177001,2.1914200874,-2.639043338 C,-4.1560134837,0.6536209219,-0.9478759431 C,-3.8110709909,2.0194606381,-1.104284781 C,-5.2309411182,0.0601299707,-1.6182721571 C,-6.0096269074,0.8423964388,-2.4677854112 P,1.2647048815,2.799755694,0.0906418901 P,-3.0986978098,-0.3506128431,0.131518495 C,-0.8838558668,1.0833069683,-0.4185635843 C,-1.2039915186,4.2386232551,0.1273987921 C,0.4998877396,1.1971557843,-0.3541918607 C,-5.075210398,-1.9656251803,1.0312843033 H,-5.579034066,-1.0227401819,1.2362919093 C,-3.7838537315,-1.9843182408,0.4872541206 C,-1.3441245012,-0.2525602475,-0.3486305344 C,-1.8644770797,5.4649222979,0.3149376031 H,-2.9485002228,5.5059447979,0.2230770548 C,-3.1009641506,-3.1975022384,0.2212774395 C,0.2050097734,4.2606136099,0.25535012 C,0.8977749837,5.4345069639,0.5922130518 H,1.9791633257,5.4266867162,0.711736243 C,-1.1843338239,6.6412766704,0.6254185917 Al,-2.1783109722,2.5547827058,-0.1254666299 C,-5.7254347332,-3.1638407288,1.310956766 H,-6.723234472,-3.1494490191,1.7377203133 C,-5.0898814689,-4.3733460788,1.0396593703 C,-3.8004641547,-4.381054969,0.5078788647 H,-3.3229397531,-5.3411312663,0.3228911731 C,0.2009311439,6.6238285348,0.7758321898 H,0.7393054819,7.5300552562,1.0347550577 Al,-1.2122272787,-3.197548149,-0.3060485417 C,-0.5252508022,-1.373792985,-0.2425589415 C,6.3964193321,-2.3507086707,0.7625045298 C,3.615083317,-2.4127004142,0.3754894633 C,4.267318899,-1.1589730923,0.4813959131 C,5.6624935129,-1.1720601111,0.6691363689 H,6.1971227688,-0.2263675951,0.7528515158 C,4.3532000085,-3.6014709415,0.5133319639 H,3.8463272924,-4.5646748989,0.4897811114 C,5.7320446485,-3.5735348033,0.6888613089 H,6.2825060851,-4.5052776873,0.780500289 P,1.7927350859,-2.6899431493,0.3411431744 C,1.4191141585,0.1266899954,-0.219780483 C,3.7768406553,2.1173176577,-0.774519336</p>

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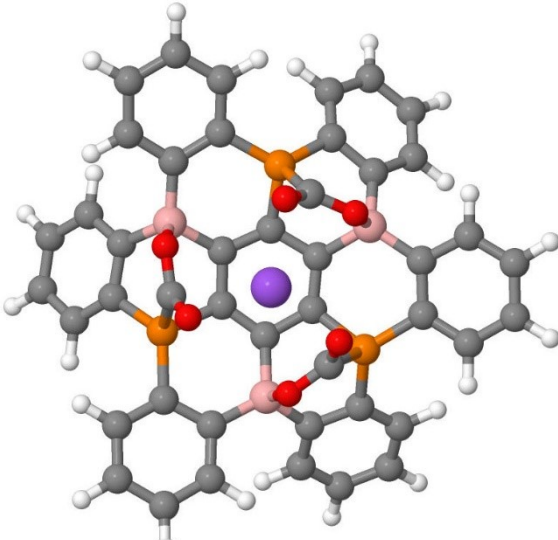
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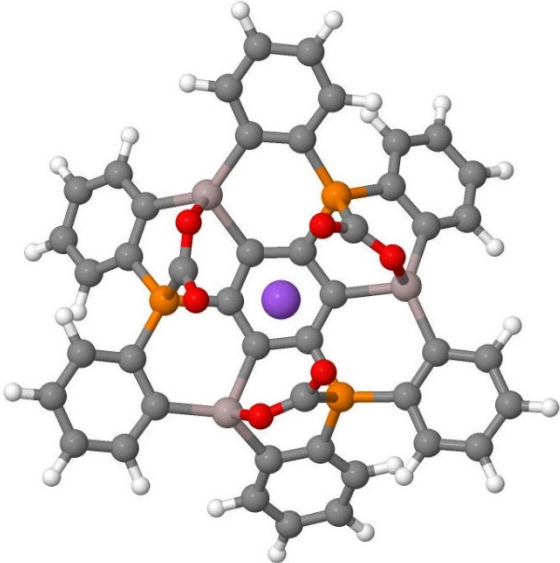


3CO₂-Al₃N₃-NG-Na

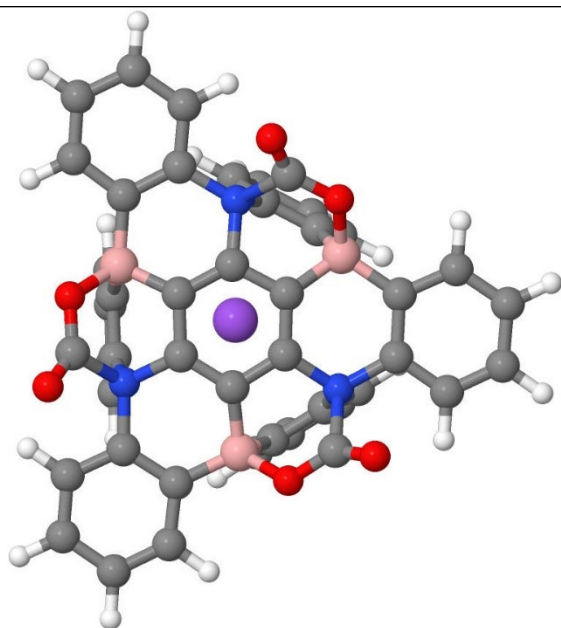
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	<p>P,-0.1718460899,-3.0318770874,0.0354071904 C,-1.2995333411,-0.6026397757,0.6474697528 C,-3.9318938655,-0.3883800809,0.9693799671 C,0.868082502,-5.1155040482,1.6396731742 H,-0.0934842533,-5.6204547561,1.6064361465 C,1.0868681688,-3.9313185316,0.9357153159 C,-0.1391462021,-1.3582954871,0.6792949408 C,-4.8963846012,-0.9885953663,1.7848862355 H,-4.9147769707,-2.0705350727,1.8857011467 C,2.3024605336,-3.2102647842,0.9699328262 C,-3.9482972696,1.0248886951,0.9340974088 C,-4.8653770052,1.8073187321,1.635952466 H,-4.8213119691,2.8924855164,1.602112642 C,-5.8319589832,-0.2273389968,2.4884335603 B,-2.762423062,-1.1490728624,0.1342609294 C,1.9053265344,-5.6252062955,2.4160316291 H,1.7639516011,-6.5460306145,2.9725979125 C,3.1135428248,-4.9334015168,2.4918394179 C,3.3047916956,-3.7438283401,1.7859925801 H,4.2510176298,-3.2184807248,1.8852058132 C,-5.8268382025,1.1648309611,2.4112034986 H,-6.5544652199,1.7482412982,2.9660407653 C,1.5909923539,4.733096403,1.7879963897 H,0.6629707997,5.2896520022,1.8887064314 H,4.9153868482,2.7289520581,1.6047276391 H,4.7892769216,4.7998091497,2.9715892511 O,-1.9567220545,1.0982434194,-2.5815616731 C,-2.456778725,0.6499589519,-1.5640556496 O,-2.7891585263,-0.5758806403,-1.3515308451 O,1.8936976492,-2.1308705223,-1.3522552942 C,0.6656808947,-2.4554370772,-1.5643789565 O,0.0272423438,-2.2468882031,-2.5819003239 O,0.8972823415,2.7054773002,-1.3509946177 C,1.7928726213,1.8051443684,-1.5642468387 O,1.931936493,1.1493794616,-2.5825853536 H,-5.3419602599,-4.9963472405,-0.937353001 H,-6.5691496162,-0.7263075522,3.1106358449 H,-1.6558947183,7.1242944994,-0.9378942638 H,2.6531010988,6.0491139229,3.1164558144 H,6.9968610201,-2.1283371054,-0.9422926715 H,3.9143732486,-5.3210835998,3.1147081016 Na,0.0027651062,-0.0007658154,-3.3229732451</p>
	<p>3CO₂-Al₃P₃-NG-Na E=-4093.32801436H; FreqIm=0 C,3.4970464943,5.1207409609,2.6348152874 C,3.0834740184,2.8869056098,1.0562107115 C,2.0592624485,3.8642178217,1.1080683925 C,4.2709737085,2.9996131927,1.7891603421 C,4.4733615408,4.1281491331,2.5791736547 P,-2.5929214389,1.6992633889,0.0669198997 P,2.7682072452,1.3960511439,0.0676232503 C,0.1388561048,1.4352816658,0.6431207481 C,-1.301117063,4.2191388219,-0.1788634511 C,-1.1028826306,0.8080847231,0.6581732854 C,5.3671520118,1.1890230391,-0.6582653003 H,5.3007711999,2.271923769,-0.7396138163 C,4.25829264,0.4272046626,-0.2551620292 C,1.2512692392,0.5511125415,0.6583335666 C,-1.403989876,5.5872166497,-0.4810164236 H,-0.5133620933,6.2113082901,-0.4367275254 C,4.304641711,-0.9824000142,-0.1781167245 C,-2.4987210042,3.4741768136,-0.2559719589 C,-3.712880605,4.0536028952,-0.659150443</p>

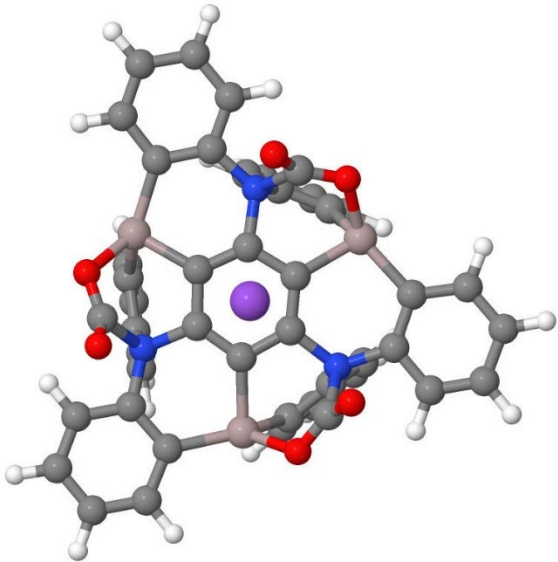
	<p> H,-4.6175494728,3.4547581848,-0.740363807 C,-2.6074502893,6.181545189,-0.8558010011 Al,0.434103398,3.3525664168,0.1121963978 C,6.5671616691,0.5548422285,-0.9575133325 H,7.4247531449,1.1421517401,-1.2699507957 C,6.6574002903,-0.8323136336,-0.8546321523 C,5.5409786186,-1.577354778,-0.4798926452 H,5.6361318213,-2.6607237954,-0.4356027541 C,-3.7636798264,5.4099416191,-0.9583955383 H,-4.7011143952,5.8590971076,-1.2706526044 Al,2.6865161715,-2.0519554259,0.1121954482 C,1.1736315503,-0.8378542457,0.6431812336 C,-4.0501161471,-5.3492251488,-0.8537655544 C,-1.7593337344,-3.9013714611,-0.255053764 C,-3.0032233558,-3.2365295762,-0.1780848951 C,-4.1367904159,-4.0096452827,-0.4796223799 H,-5.1225413415,-3.5502896571,-0.4350172664 C,-1.6544424573,-5.2428029422,-0.6577160983 H,-0.6835670137,-5.7270354889,-0.7389584978 C,-2.8038422624,-5.9649321866,-0.9564677454 H,-2.7243139326,-7.0014869098,-1.2683215849 P,-0.1748781126,-3.095520765,0.0674872362 C,-1.3123379381,-0.5973907747,0.6430505662 C,-4.3761310704,-0.1485427309,1.1073163235 C,0.4625663407,-5.1983836123,1.7892432404 H,-0.5902031842,-5.4645757118,1.7588592009 C,0.9586675548,-4.1137364594,1.0561351675 C,-0.1482499437,-1.3592360045,0.6581354878 C,-5.4676094103,-0.4901886309,1.9153380708 H,-5.7687845362,-1.5324439999,1.9959831169 C,2.3171380824,-3.7153303023,1.1078400768 C,-4.0418230104,1.2270875709,1.0554062537 C,-4.7332728438,2.1992584774,1.7880013205 H,-4.4374808435,3.2441026122,1.7567684011 C,-6.1833419953,0.4687191632,2.6339070481 Al,-3.1203708465,-1.3003503776,0.1119899981 C,1.3387983763,-5.9382354591,2.5787378393 H,0.9659571315,-6.7819677252,3.150878712 C,2.6865835251,-5.5891328244,2.6342359572 C,3.1588668609,-4.4896418158,1.9158567575 H,4.2121916989,-4.2296345288,1.9960316265 C,-5.8118864503,1.810516613,2.5779125255 H,-6.3560577303,2.5553634224,3.1500257163 C,2.3090578025,4.9803501404,1.91593968 H,1.5571790177,5.7625002651,1.996063108 H,5.0282353316,2.221278761,1.7579498679 H,5.3903154709,4.22697433,3.1515926496 O,-1.8793874614,1.1933294742,-2.4815259786 C,-2.5727712311,0.7330878246,-1.5873000626 O,-3.1283960166,-0.4175941304,-1.5453260776 O,1.9257801632,-2.5002356501,-1.5450276156 C,0.6513884965,-2.5949824356,-1.5867041298 O,-0.09428455,-2.2251367348,-2.4808533499 O,1.2027490294,2.9180592495,-1.5449724562 C,1.9216107611,1.8616165598,-1.5868494104 O,1.9737416619,1.0310551845,-2.4811471385 H,-4.9521681654,-5.910018162,-1.0802767863 H,-7.0271998348,0.1678622178,3.2481101308 H,-2.6421692449,7.2429868561,-1.0829613671 H,3.6582816097,6.0020706149,3.2489195868 H,7.5940072998,-1.3329700574,-1.0817251366 H,3.3692949358,-6.1696938574,3.247974513 Na,0.0003667688,-0.000807479,-3.1903792981 </p>
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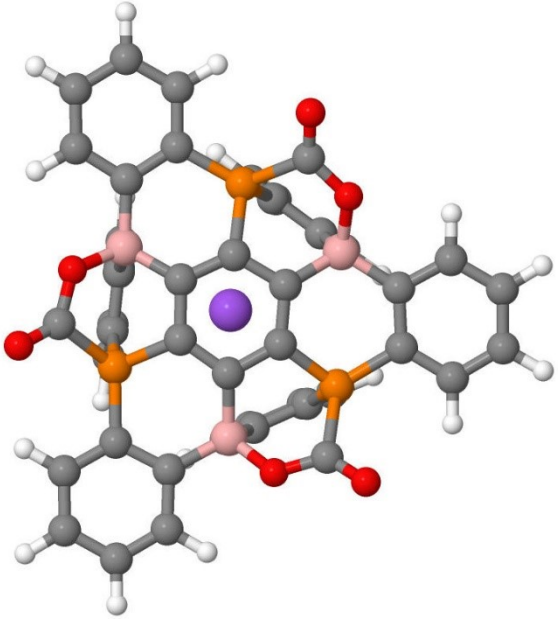


3CO₂-B₃N₃-NG-Na down

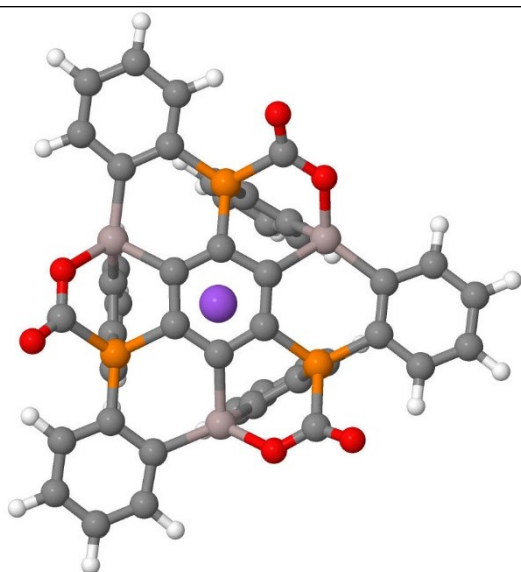
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 C,-1.5299051025,2.8738681419,1.8614617063
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 N,-1.410312027,2.4086620747,-0.6282391608
 C,-1.4027008375,0.0299873289,-1.0212835519
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 H,2.4384251654,5.068899007,-0.6110926073
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 C,4.9177014721,-1.2012179511,-0.6677494186
 H,5.4144229201,-0.237598041,-0.6665420584
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 H,-2.7985454442,-2.7023205811,1.7533034204
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 H,1.5428772943,3.3659403925,2.2670785284
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	<p>H,-0.9425234868,3.778303893,1.7481496382 H,-1.6339456754,3.019072354,4.0045172658 O,-1.4148925767,-4.0427630906,-2.4634044358 C,-0.6826216444,-3.5499833942,-1.6805076417 O,0.5677279107,-3.6519239373,-1.4565716611 O,2.8780482907,2.3170830927,-1.4602215275 C,3.4149418095,1.1833086081,-1.6842821834 O,4.2071527187,0.7953535691,-2.4677406312 O,-3.4457685404,1.3331284755,-1.4602523219 C,-2.7323243008,2.3647888506,-1.6852240723 O,-2.7924133682,3.2441550976,-2.469473023 H,5.6410969324,-4.5184946241,-0.6408088437 H,0.6693989553,-3.0668173269,4.2772201735 H,-6.7330455388,-2.6260481906,-0.6314516866 H,-2.9932354123,0.9596708818,4.2740883327 H,1.0931332405,7.1439582504,-0.6408089483 H,2.3266829489,2.1158922869,4.2737810446 Na,-0.0013543733,0.0018273673,1.9227232784 B,-2.893124762,0.2044143716,-0.5555029165 B,1.2698883324,-2.6081729567,-0.5537959071 B,1.6235932485,2.403338494,-0.556596325</p>
	<p>3CO₂-Al₃N₃-NG-Na down E=-3233.43392377H ; FreqIm=0</p> <p>C,-1.2097156016,-2.8737468902,3.5260664595 C,-1.8223448721,-2.3638229575,0.8536455366 C,-0.6447372787,-3.0818248005,1.1485199411 C,-2.6816110839,-1.9133428973,1.8612651705 C,-2.3628363438,-2.1664607696,3.1982807618 N,2.7165512566,-0.8606736246,-0.5822140408 N,-2.102089048,-1.9223078353,-0.5821904675 C,0.2665415213,-1.3940375449,-0.9032277654 C,2.407657486,-3.4483121669,-0.6877936641 C,1.2751954073,-0.46382039,-0.8899802806 C,-4.3414324743,-2.7979542414,-0.7613802427 H,-3.8566270947,-3.7714893815,-0.7447859234 C,-3.5777186899,-1.6281025052,-0.7236559587 C,-1.0382948052,-0.8718779382,-0.8885232754 C,3.0963701683,-4.6763091746,-0.7537663988 H,2.5232119765,-5.6005104298,-0.7403434215 C,-4.1884068823,-0.3605113118,-0.6808329884 C,3.2000752254,-2.2853539369,-0.7264223597 C,4.5949899784,-2.3615585596,-0.7627851824 H,5.1957270384,-1.455009052,-0.7432993232 C,4.4807768865,-4.7624728388,-0.8278360856 Al,0.4836073561,-3.2691970367,-0.4603306264 C,-5.7261667276,-2.7376881545,-0.8143838614 H,-6.3010781417,-3.6571985671,-0.8552983252 C,-6.3635080434,-1.4983553581,-0.8192155256 C,-5.5964351126,-0.3427630616,-0.7441388619 H,-6.1102180603,0.6156598885,-0.7275662868 C,5.2352784762,-3.5907562376,-0.8188608268 H,6.3190819505,-3.6286852848,-0.8591146115 Al,-3.0709660235,1.216091356,-0.4532905361 C,-1.3393695637,0.4668750165,-0.8998160865 C,1.8868562364,6.2601069992,-0.8257516609 C,0.3804052671,3.9131391818,-0.7255230233 C,1.7835990589,3.8079868098,-0.6818499519 C,2.5036156908,5.0179618554,-0.7472634827 H,3.5905046383,4.9831994297,-0.7299164049 C,-0.2502471804,5.1595144069,-0.7669995311 H,-1.3357032086,5.2272404577,-0.7515127181 C,0.494903373,6.3281892876,-0.8223628606 H,-0.0136868261,7.2858232048,-0.8665843576</p>

	<p>N,-0.6121971794,2.7827879381,-0.5809979577 C,1.075047921,0.9273398067,-0.9019710823 C,2.9870558116,0.976678463,1.1538667569 C,-0.313690384,3.2874697253,1.8608686986 H,0.6071623646,3.8103489186,1.6308153996 C,-1.132887966,2.7636505361,0.8553462322 C,-0.2349189881,1.3361076546,-0.8873279681 C,3.0581059464,1.3298304951,2.5089418442 H,3.0891837189,2.3840989118,2.776958817 C,-2.3426974899,2.1025368311,1.1529265976 C,2.9551606255,-0.4014517783,0.855389678 C,2.9914008757,-1.3735589422,1.8605018626 H,2.9840805468,-2.4323162199,1.6296211553 C,3.0802954076,0.3770196521,3.5302528799 Al,2.5892801342,2.0518851696,-0.4535330649 C,-0.6919009826,3.1427424753,3.1984045317 H,-0.0521496897,3.5521717878,3.974405697 C,-1.8800824385,2.4975372418,3.5288559877 C,-2.6892972984,1.9948636006,2.5072605953 H,-3.6186654218,1.4956703505,2.7744052587 C,3.0460574474,-0.9744505654,3.1988369335 H,3.0743207633,-1.7336138361,3.9746932318 C,-0.3738903234,-3.3262226939,2.5023829724 H,0.5237002372,-3.8815414837,2.7674654705 H,-3.5946073195,-1.3760628636,1.6332111278 H,-3.0342057046,-1.8148564373,3.9759300025 O,3.6614174031,-0.6565795549,-2.8309774862 C,3.5483804945,0.0117673722,-1.8690728882 O,3.8239546791,1.1932600495,-1.530826187 O,-2.9432506252,2.7120065721,-1.5349271541 C,-1.7822949836,3.0649644542,-1.8715737962 O,-1.2577658436,3.4960165933,-2.8326316351 O,-0.8776829433,-3.904787822,-1.5398116826 C,-1.7642843676,-3.0749180897,-1.8736219148 O,-2.4013888647,-2.8357141896,-2.8336091487 H,2.4816223537,7.1666568957,-0.8774586746 H,3.1325171799,0.6854570689,4.5702872612 H,4.9691014354,-5.7304700565,-0.8805268402 H,-0.9684579618,-3.0780032283,4.5651080669 H,-7.4460831721,-1.4368948272,-0.8692870237 H,-2.1774633492,2.3945854156,4.5683170707 Na,0.0088679113,-0.0081538382,1.7083842027</p>
	<p>3CO₂-B₃P₃-NG-Na down E=-3440.60555839H; FreqIm=0 C,0.0077805538,-2.8996861569,3.2988819738 C,-1.4303381466,-2.4985715693,0.9809249316 C,-0.063860986,-2.8431566433,0.860320368 C,-2.0860280505,-2.3857603746,2.2048782287 C,-1.3470648456,-2.5725137343,3.3786008378 P,2.9421968663,-0.8064723871,-0.6413045462 P,-2.1699028225,-2.1442023629,-0.6435411954 C,0.3164652796,-1.3914455165,-1.1971477373 C,2.0838508775,-3.4177964754,-0.7458492619 C,1.3001164115,-0.4141597257,-1.2240516961 C,-4.9015406051,-2.4075611982,-0.7346837207 H,-4.7189391264,-3.4794393154,-0.7332172611 C,-3.8304604163,-1.5023027479,-0.6972993902 C,-1.0089938005,-0.9178613343,-1.2256264542 C,2.3604788922,-4.7885886216,-0.8278925474 H,1.5269574918,-5.4839004176,-0.8851359058 C,-4.0021221455,-0.0954690964,-0.7465952281 C,3.2162800565,-2.5657714438,-0.6951465732 C,4.5358266692,-3.0407578931,-0.7334760773</p>

	<p> H,5.3728566558,-2.3466997765,-0.7316497592 C,3.6657181189,-5.2788800297,-0.8591064791 B,0.5538801659,-2.9125300104,-0.6739691673 C,-6.1980698689,-1.9142632166,-0.8106562312 H,-7.0382169544,-2.5998036065,-0.8486701084 C,-6.4049055114,-0.5348758865,-0.8571946432 C,-5.3277172835,0.3503522892,-0.8266678524 H,-5.5133581312,1.4198767745,-0.8830192997 C,4.7568938861,-4.4101314209,-0.8112385374 H,5.7706707237,-4.7948974001,-0.8497258489 B,-2.799660208,0.9770489646,-0.6749055271 C,-1.3635721028,0.4227828766,-1.1982552455 C,2.739229788,5.8146162278,-0.8618277393 C,0.6141658254,4.0692269006,-0.6973337293 C,1.9184123658,3.5143858188,-0.7452073791 C,2.9672550095,4.4392369955,-0.8271174625 H,3.9862951228,4.0650268425,-0.8817407814 C,0.3656993096,5.4492923038,-0.7393651166 H,-0.6539282575,5.8270701052,-0.7396993061 C,1.4411501931,6.3252797422,-0.8176892556 H,1.2674773733,7.395470804,-0.8597373605 P,-0.7723183755,2.9521770477,-0.6433381669 C,1.0475450509,0.9705377805,-1.1964295451 C,2.4933539905,1.367580975,0.8616282371 C,-1.0223350214,2.9958562594,2.205507369 H,-0.2894061254,3.7979676862,2.2492905535 C,-1.4488627757,2.48721423,0.9808330038 C,-0.2906669539,1.333876051,-1.2255208763 C,2.3225612314,2.0768101524,2.0543400924 H,2.0609676048,3.1320299398,2.0111882198 C,-2.4307537535,1.4762411629,0.8592106804 C,2.8786020848,0.0119505636,0.9828550749 C,3.1090060231,-0.6111739312,2.2072397182 H,3.4377038854,-1.6468450088,2.2504865573 C,2.5074647848,1.4596911211,3.3001407362 B,2.2459070706,1.9368350379,-0.672291609 C,-1.5536504683,2.4478215281,3.3786699954 H,-1.2333154101,2.8226214288,4.3460957818 C,-2.5153665845,1.4390256589,3.2976710706 C,-2.9587698986,0.9720976328,2.0515403771 H,-3.7412813112,0.2173752466,2.0078142066 C,2.9018176559,0.1229521413,3.3806769164 H,3.0693738605,-0.3410833615,4.3479221773 C,0.6354998621,-3.0488824253,2.0533901961 H,1.6805206697,-3.348863844,2.0109367226 H,-3.1473083492,-2.1521255579,2.2478001971 H,-1.8331538208,-2.4844699219,4.3455218284 O,5.0387393712,0.100351295,-2.1380211707 C,4.0376297465,0.4368814487,-1.5738055879 O,3.5230951455,1.6304984848,-1.4638269504 O,-3.1730483883,2.2362669425,-1.4662887208 C,-2.3963962933,3.2785257672,-1.5765019808 O,-2.6054218245,4.3135339932,-2.1411894346 O,-0.3496207693,-3.8649953122,-1.4663610442 C,-1.6406440336,-3.7141964313,-1.5758397983 O,-2.4323773917,-4.4120782971,-2.1414486034 H,3.834119671,-6.3493680862,-0.9319933322 H,3.58220195,6.495558676,-0.9346306913 H,-2.941860126,1.0299456212,4.2096419182 H,-7.4162722014,-0.1454092712,-0.9279060451 H,0.5742255644,-3.0651241179,4.2113984541 H,2.3684562862,2.0338478408,4.2122657974 Na,-0.0039420067,-0.0019894304,1.8985417604 </p>
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3CO₂-Al₃P₃-NG-Na down

E=-4093.30831740H; FreqIm=0

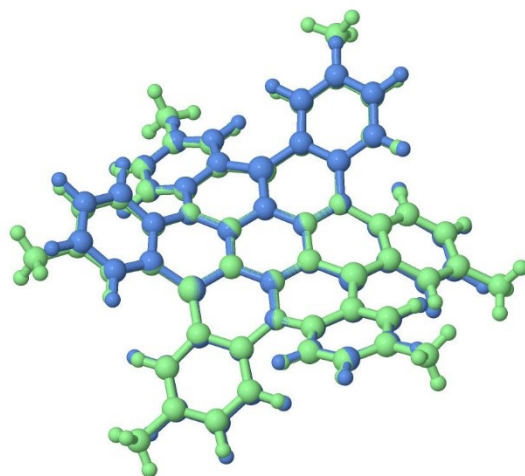
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 C,-0.6033854941,-2.854998638,1.2117769226
 C,-2.7420732124,-1.9419265685,2.060758051
 C,-2.2762891182,-2.0533121684,3.3742786136
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 P,-2.4021002103,-2.0096506796,-0.7288222517
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 C,2.2617670907,-3.8084325015,-0.6166802287
 C,1.2705788962,-0.5105746442,-1.2424271008
 C,-5.0934858354,-2.4102329027,-0.9555914841
 H,-4.823611592,-3.4486834504,-1.116287627
 C,-4.1086123398,-1.4226304785,-0.809321592
 C,-1.0782224519,-0.8441944179,-1.2437004778
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 H,1.92645391,-5.934081286,-0.4726339477
 C,-4.4304745824,-0.054074553,-0.6184971267
 C,3.2864807461,-2.8453269006,-0.8044267824
 C,4.6345550891,-3.2042843453,-0.947095294
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 C,4.0077862977,-5.522867113,-0.742844756
 Al,0.3794181619,-3.2702371367,-0.5027533318
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 H,-7.2019481028,-2.8031895206,-1.0490182954
 C,-6.7881226694,-0.7085893333,-0.7479947064
 C,-5.7967957034,0.2625917809,-0.5981172868
 H,-6.1037537285,1.298720366,-0.4718440598
 C,4.9887289583,-4.550901347,-0.9162678716
 H,6.0295221097,-4.8335915836,-1.0374959619
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 C,-1.3389495339,0.5266754733,-1.2286839697
 C,2.7793590363,6.2338879986,-0.7479385237
 C,0.820906992,4.2707386077,-0.8080114869
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 C,3.1246407206,4.8897283031,-0.5983177677
 H,4.1754637455,4.6372905657,-0.4727222726
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 H,-0.576161368,5.9034070517,-1.1139250064
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 H,1.1722237943,7.6398316018,-1.0475485489
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 C,1.124650081,0.897111207,-1.2271051628
 C,2.7708359152,0.9079151293,1.2144455517
 C,-0.307957074,3.3389157086,2.0609100724
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 C,-0.1928519282,1.3569056713,-1.2443544933
 C,2.6520751022,1.321895157,2.5494973042
 H,2.5217171249,2.3795990968,2.7710324722
 C,-2.1714062873,1.9480591161,1.2115264578
 C,2.9580844644,-0.4843196946,1.0133744332
 C,3.0535731451,-1.400204598,2.0641787826
 H,3.2239090332,-2.4568593037,1.867398683
 C,2.7089901882,0.4157192979,3.618334291
 Al,2.6413892194,1.9656640429,-0.5012019557

	C,-0.634009414,2.9866338801,3.3739823603 H,-0.0567251048,3.389016275,4.2012772368 C,-1.7063020845,2.1297124372,3.6147689407 C,-2.4672646839,1.6335303339,2.5462288346 H,-3.318740028,0.9926939064,2.7677896082 C,2.9175035405,-0.9409687147,3.3775847704 H,2.9838168862,-1.6412180226,4.2051400523 C,-0.1854139304,-2.9588657678,2.5468046983 H,0.7950961735,-3.3762369058,2.7684396694 H,-3.7415247439,-1.5590868631,1.8637547969 H,-2.9151951698,-1.7584721323,4.2016079084 O,5.0616976928,-0.5127419887,-2.3296903547 C,4.233973514,0.0232235849,-1.6494330101 O,4.0570097741,1.282855239,-1.4163462939 O,-3.1387533152,2.87227562,-1.4209881683 C,-2.1377402104,3.6576240252,-1.651262819 O,-2.0888503428,4.644700965,-2.3283483371 O,-0.9183750627,-4.1536354439,-1.4211043308 C,-2.0972505088,-3.6762550863,-1.6548499855 O,-2.9748057644,-4.1240650314,-2.3364391296 H,3.5525809422,6.9963279159,-0.7314381439 H,2.6121169745,0.7749525612,4.6393829947 H,4.2817593212,-6.5736332169,-0.7256760486 H,-0.6384362158,-2.6483552632,4.6365550451 H,-7.8351036491,-0.4204898911,-0.7308730403 H,-1.9662984743,1.862861927,4.6356201023 Na,-0.0033830031,0.008366597,1.6961037311
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Table S9. Energy partition terms (kJ mol⁻¹)

NG	Adduct	$\Sigma E_{\text{def}}(i)$	$\Sigma \Sigma \Delta^2 E(ij)$	C
Al ₃ N ₃	1CO ₂ -NG	+335.8	-331.8	-
	2CO ₂ -NG	+523.6	-512.0	-5.8
	3CO ₂ -NG	+809.7	-792.2	-21.6
B ₃ P ₃	1CO ₂ -NG	+408.0	-415.3	-
	2CO ₂ -NG	+841.3	-850.9	-24.1
	3CO ₂ -NG	+1293.4	-1293.3	-80.4
Al ₃ P ₃	1CO ₂ -NG	+250.4	-349.5	-
	2CO ₂ -NG	+655.4	-870.4	-8.1
	3CO ₂ -NG	+1009.8	-1343.4	-26.9

Figure S1. Overlap of the optimized geometry of B3N3-NG (blue) and CSD refcode FEWKIE (green).



Jmol

Figure S2. Free energy profiles of the capture of one CO₂ molecule by the B₃N₃-NG, B₃P₃-NG, Al₃N₃-NG and Al₃P₃-NG systems at M06-2X/6-311++G(3df,3dp)//M06-2X/6-31+G* level of theory.

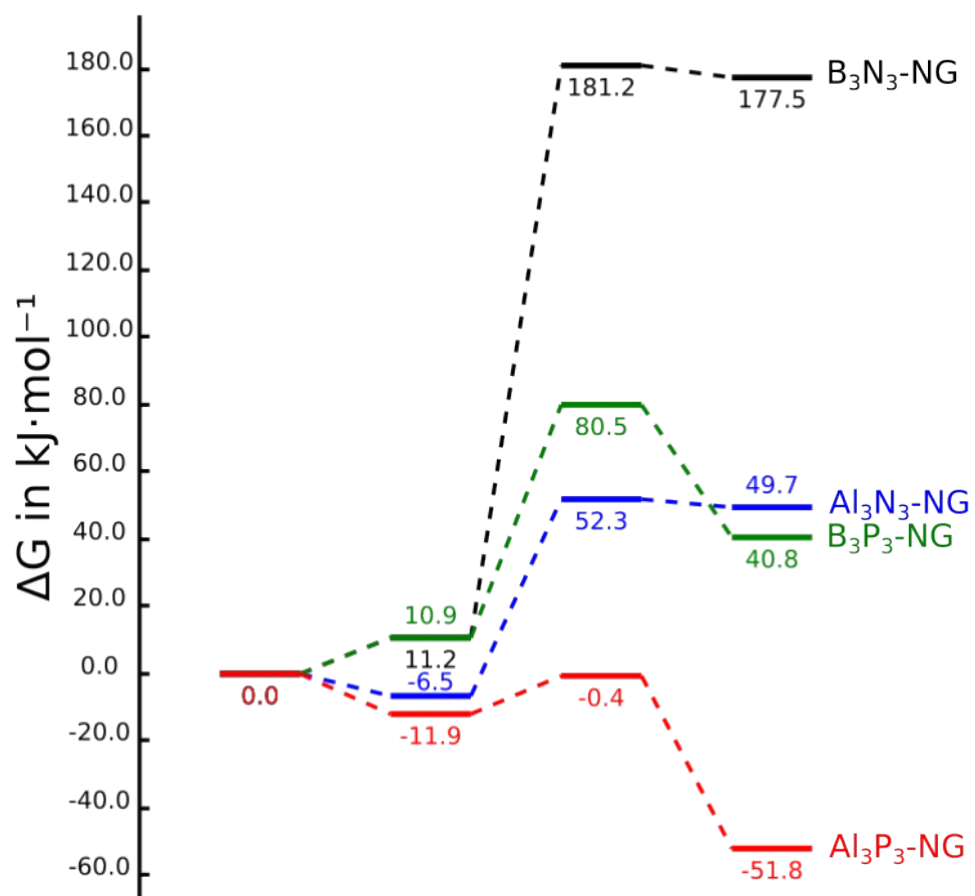


Figure S3: Exponential correlation of the six BCP's obtained for the Al-O and C-P contacts vs. the interatomic distances.

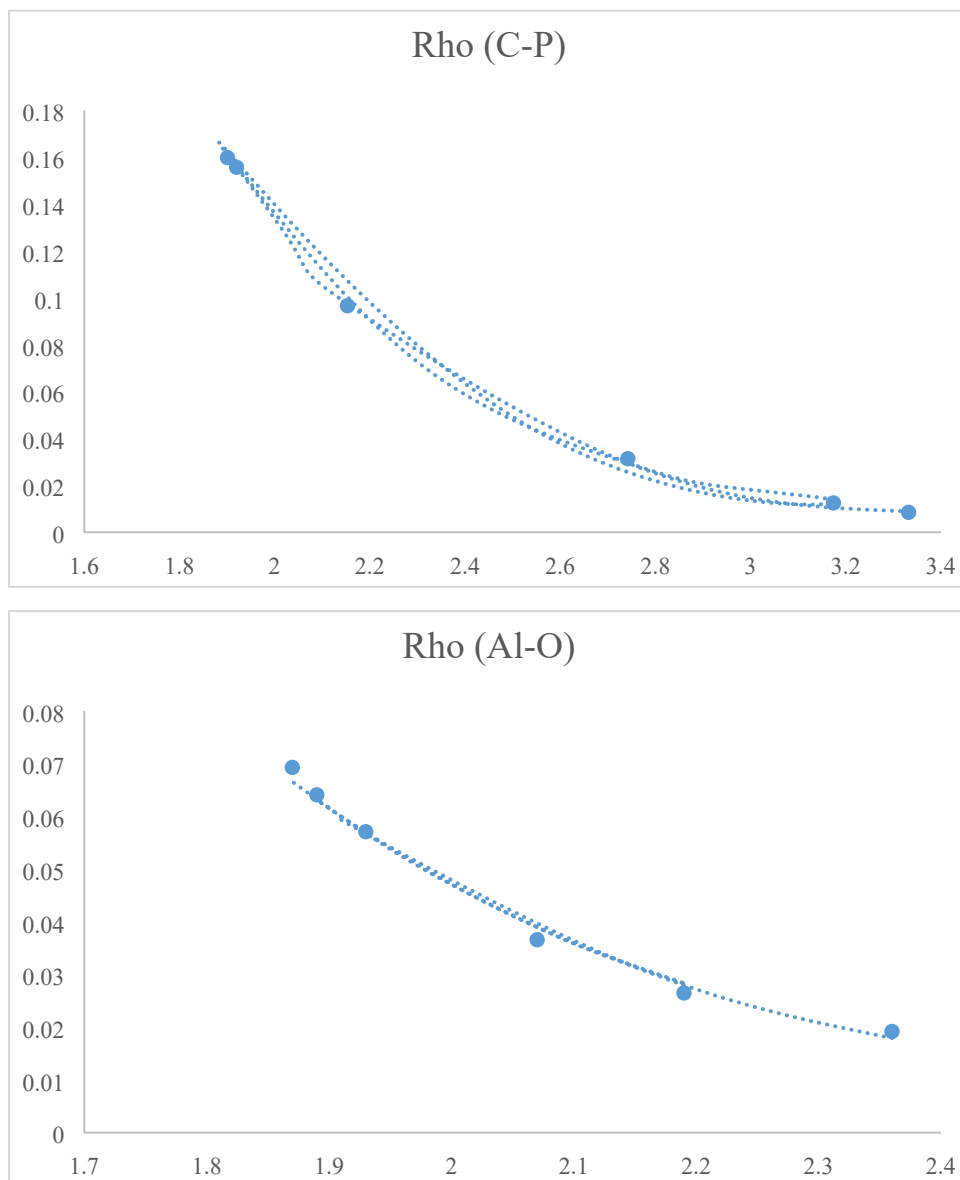


Figure S4: Superposition of the NG-Na-up (blue), NG-Na-low (green) and NG (yellow) geometry, along with the decomposition of the binding energy ($E_b = E_{def} + E_{interaction}$) in kJ/mol.

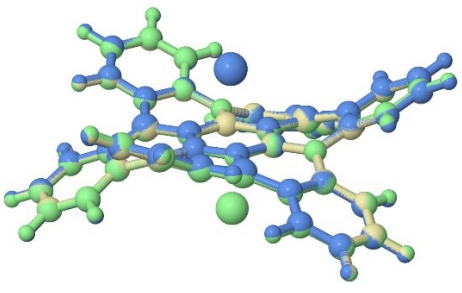
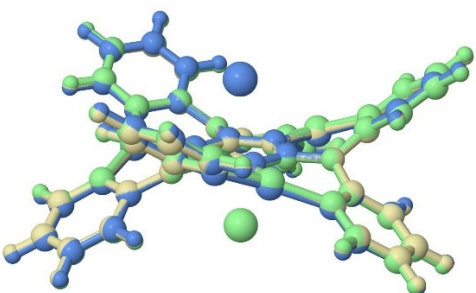
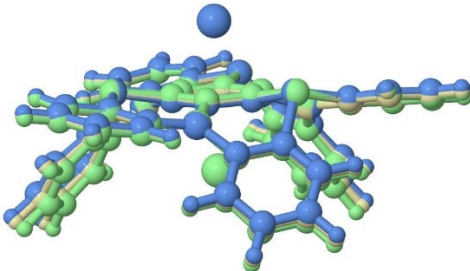
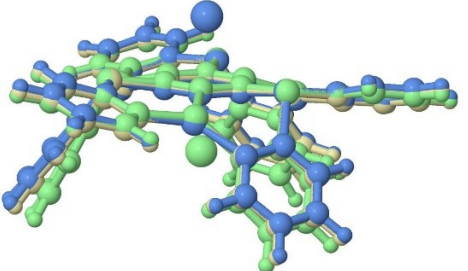
	<i>B₃N₃-NG</i>	<i>Al₃N₃-NG</i>
		
E_b (NG-Na-up)	-166.8	-200.3
EDA	=3.5+(-170.3)	=7.9+(-208.2)
E_b (NG-Na-low)	-166.8	-200.2
EDA	=3.5+(-170.3)	=7.8+(-208.2)
	<i>B₃P₃-NG</i>	<i>Al₃P₃-NG</i>
		
E_b (NG-Na-up)	-175.3	-193.8
EDA	=3.5+(-178.9)	= 5.8+(-199.5)
E_b (NG-Na-low)	-182.6	-185.4
EDA	=5.0+(-187.9)	=15.0+(-200.4)

Figure S5: Comparative energy profiles of the reaction of B₃N₃-NG and B₃P₃-NG in the absence/presence of Na⁺ with three molecules of CO₂.

