

Supporting Information Material

Theoretical study of the reaction of borata derivatives of  
benzene, anthracene and pentacene with CO<sub>2</sub>

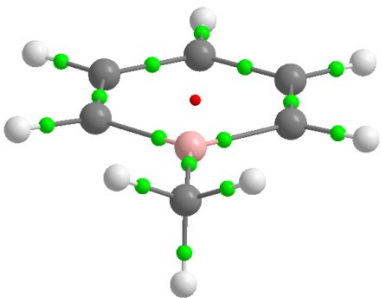
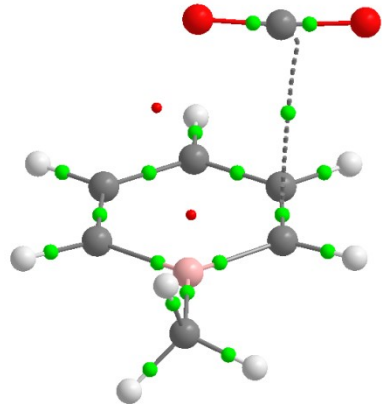
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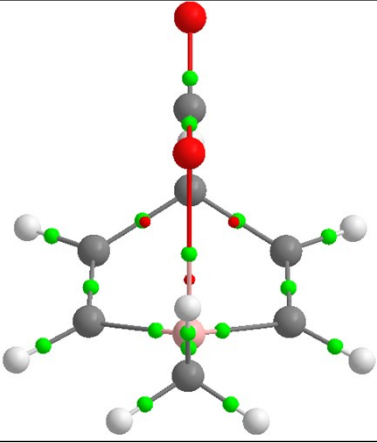
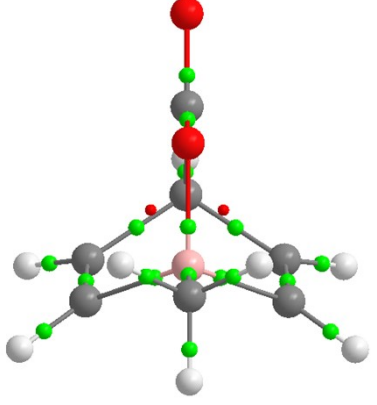
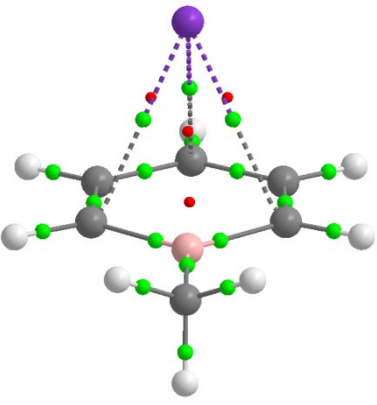
- Pg. S2-58 Table S1. Molecular graph, electronic energy (hartree) and cartesian coordinates (Å) of the stationary points.
- Pg. S59 Table S2. Comparison of the relative energies (kJ mol<sup>-1</sup>) of eight minima calculated at the M06-2X/def2TZVP, PBE0-D3/def2TZVP and DLPNO-CCSD(T)/def2TZVP computational levels. The differences with respect to M06-2x calculations are shown in parenthesis.
- Pg. S59 Table S3. Comparison of the relative energies (kJ mol<sup>-1</sup>) computed with the SMD implicit solvent model and with two THF molecules interacting with the potassium cation and the SMD model. Energy differences are shown in parenthesis.
- Pg. S59 Table S4. Bond distances (Å) of the 1methyl-boratabenzene.
- Pg. S60 Fig. S1. Energy profiles for the reactions **BBZN** + CO<sub>2</sub> → **BBZN-CO<sub>2</sub>** (left) and **BBZN-K** + CO<sub>2</sub> → **BBZN-K-CO<sub>2</sub>** (right) with the corresponding molecular graphs of the stationary points. Green, red and blue small spheres indicate the location of the bond, ring and cage critical points.
- Pg. S61 Fig. S2. X-ray structures of the 9-borataanthracenes refcodes GAFXUG and GAGGIE and the calculated 9-methyl-9-borataanthracene anion and its potassium salt. The bond distances (Å) of the central ring are indicated.
- Pg. S62 Fig. S3. Energy profiles of reactions **BA** + CO<sub>2</sub> → **BA-CO<sub>2</sub>** (left) and **BA-K** + CO<sub>2</sub> → **BA-K-CO<sub>2</sub>** (right) with the molecular graphs of the stationary points.
- Pg. S63 Fig. S4: Optimized geometry of BA:CO<sub>2</sub>, BA-K:CO<sub>2</sub>(1) and BA-K:CO<sub>2</sub>(2) complexes (M06-2X/def2TZVP).
- Pg. S64 Fig. S5: Superposition of the crystal (green) and optimized (blue) structures of the diboratapentacene derivatives. The corresponding CSD refcode used is indicated.
- Pg. S65 Fig. S6: Scan of the two CO<sub>2</sub> angle capture by the trans-DBP calculated at M06-2X/def2SVP level.
- Pg. S66 Fig. S7. Free energy profile (kJ mol<sup>-1</sup>) of the formation of the syn adducts with two CO<sub>2</sub> molecules
- Pg. S67 Fig. S8. Reaction profile of *cis*- (green) and *trans*-DBP-K (black) with two CO<sub>2</sub> molecules.
- Pg. S68 Fig. S9. Syn products of the addition of two CO<sub>2</sub> molecules to the *cis* and *trans*-DBP-K molecules.
- Pg. S69 Fig. S10. Solvation thermodynamic cycle and the energetic relations derived from them.
- Pg. S70 Fig. S11. MEP of the *trans*-diboratapentacene in the presence of two potassium cation atoms and two 18-crown-6-ether molecules and the analogous systems with the adduct of one CO<sub>2</sub> molecule. The geometry and wavefunction of these systems corresponds to M06-2X/def2svp calculations.

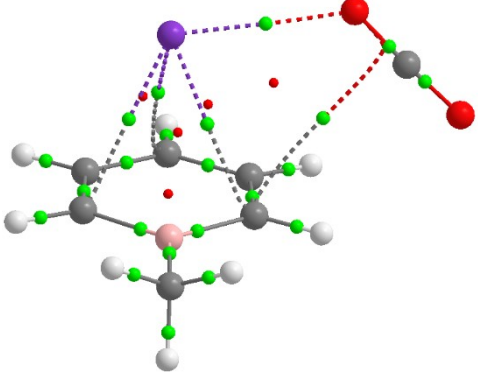
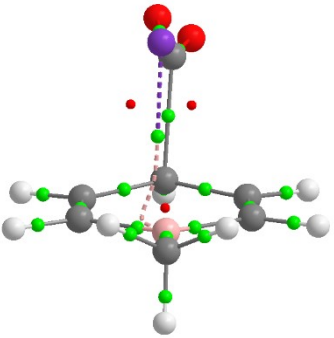
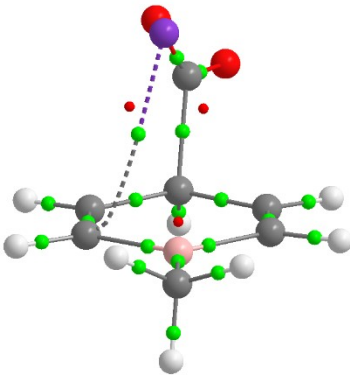
Table S1. Molecular graph, electronic energy (hartree) and cartesian coordinates (Å) of the stationary points.

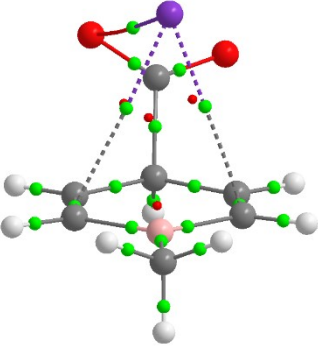
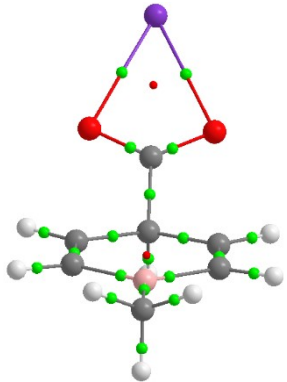
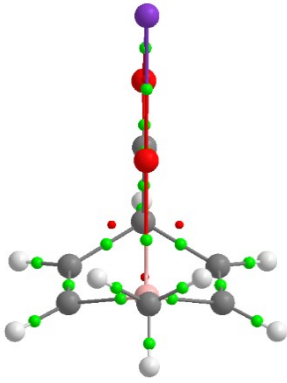
Nomenclature used for the systems is: **BBZN**: 1-methylboratabenzene, **BA**: 9-methyl-9-borataanthracene, **cis-DBP**: 5,7-dimethyl-5,7-diboratapentacene and **trans-DBP**: 5,12-dimethyl-5,12-diboratapentacene.

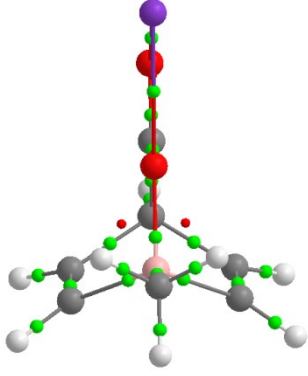
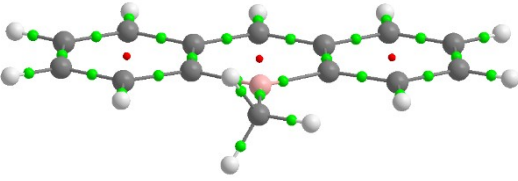
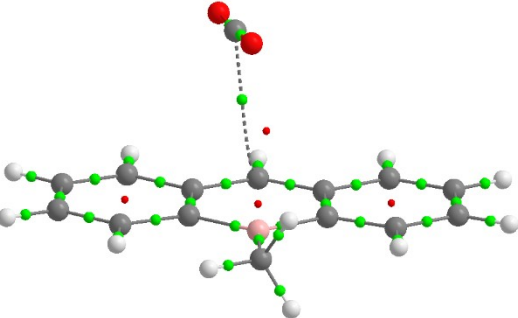
The complexes are identified with “:”, for instance BBZN:CO<sub>2</sub>, transitions states with “/”, for instance BBBZ/CO<sub>2</sub>, and the adducts with “-”, for instance BBZN-CO<sub>2</sub>.

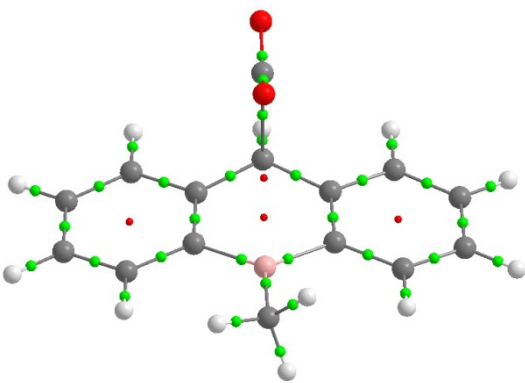
<b>Boratabenzene<sup>(-)</sup></b>	
BBZN ; E= -258.318587741H  	15 C,0.6535545933,-1.1234620003,-0.8304521215 C,0.7089347406,0.1351058078,-1.4189103826 C,-0.3280258877,1.0656583386,-1.2958614108 C,-1.4762439087,0.7451887096,-0.5642472463 C,-1.6385931241,-0.4835134165,0.0660362267 H,-0.2441401961,2.0363873448,-1.7743313664 B,-0.5547529976,-1.5349808074,-0.0191645779 C,-0.6689967714,-2.9691451187,0.712563426 H,-0.259839732,-2.9285610566,1.7294180878 H,-1.7058807047,-3.309015669,0.8103150898 H,-0.1134015107,-3.7537460141,0.1872839918 H,1.5152555384,-1.7741319606,-0.9942997616 H,1.5816743299,0.4269822717,-2.0046286596 H,-2.2613431809,1.4999195731,-0.5015421233 H,-2.5762584505,-0.6318582662,0.6059673603
BBZN:CO <sub>2</sub> ; E= -446.926054326H  	18 C,0.6420801563,-1.1361927856,-0.8543013873 C,0.6947061418,0.1242030792,-1.4495075315 C,-0.3258374102,1.0649978764,-1.2978553931 C,-1.4636222943,0.7525146127,-0.5412195064 C,-1.6261479919,-0.4748708286,0.0841716526 H,-0.2433134626,2.0356506353,-1.7761455212 B,-0.5527956713,-1.5382474559,-0.0218507571 C,-0.6678005847,-2.9675861471,0.7151678748 H,-0.4506746365,-2.8786488654,1.7864643454 H,-1.6748663401,-3.392788568,0.642844516 H,0.0314658552,-3.7079611511,0.3125373491 C,2.0384848493,0.6934499399,1.1870087739 O,1.0913559282,0.9384487955,1.7967188876 O,3.0517207679,0.4969664603,0.6587526687 H,1.4965190015,-1.7913419932,-1.0345163159 H,1.5589553128,0.4062468574,-2.0513781693 H,-2.2357551172,1.5174015452,-0.4540308562 H,-2.5509702142,-0.6125490769,0.6477662299
BBZN/CO <sub>2</sub> ; E= -446.899499829H	18 C,0.6715434231,-0.2534882711,1.4973702837 C,-0.5795550712,-0.6990971142,1.3247880247 C,-1.0874471774,-0.914417198,-0.0543302065 C,-0.0868512636,-1.4958070426,-0.985500112 C,1.1860196449,-1.0854045154,-0.9150063732 H,-2.0568324053,-1.4016528672,-0.0930417441 C,2.6958956313,0.9965346133,0.0935051608 H,3.1394789612,1.2358815844,1.0639812964

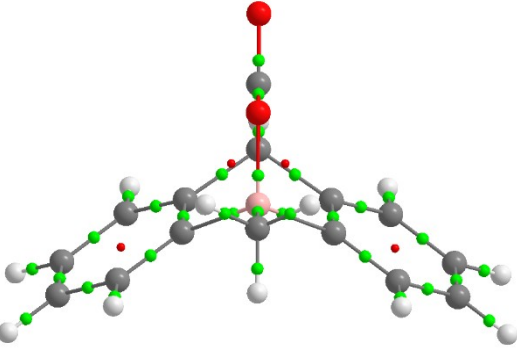
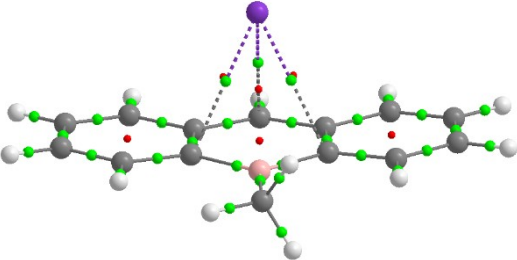
	<p>H,3.4905362783,0.6681453267,-0.5821998223  H,2.2865647804,1.9260373719,-0.3143550656  O,-0.288850902,1.3046693592,-0.6492785548  C,-1.3226340982,0.6259128663,-0.6356740031  O,-2.4812983762,0.8695955148,-0.9668076122  B,1.490031922,-0.0261396937,0.1890297576  H,1.0177003185,0.01421228,2.4930766233  H,-1.2953887321,-0.787461573,2.1383608159  H,-0.4599083835,-2.1384443959,-1.7792080852  H,1.9036844496,-1.4184362455,-1.6613083835</p>
<p>BBZN-CO<sub>2</sub> ; E= -446.924379854H</p> 	<p>18  C,-0.6987415679,1.2939855447,0.635267485  C,-0.863857744,1.2519848506,-0.6833594929  C,-0.3048725804,0.0007730125,-1.3571916611  C,-0.8694647536,-1.2480068061,-0.683497517  C,-0.7045796037,-1.2908998485,0.6351294396  H,-0.4119631291,0.001069766,-2.4384801052  C,0.5979783409,-0.0015187604,2.7242762055  H,-0.2705160617,0.000417766,3.3924078271  H,1.1964599777,-0.8850796394,2.9693607774  H,1.200466705,0.8792884786,2.9694551229  O,1.4122575756,-0.0032608106,0.2792358986  C,1.1968264943,-0.0025596446,-1.0034479863  O,2.0685607662,-0.0047253728,-1.8532737407  B,0.1363844444,-0.0003871326,1.1821709025  H,-1.0608718172,2.1372483519,1.2198172002  H,-1.3209739541,2.0175038366,-1.3038065361  H,-1.33000975,-2.0113951871,-1.3040344657  H,-1.0705012078,-2.1325946769,1.2195782686</p>
<b>Borabenzene<sup>(-):K<sup>(+)</sup></sup></b>	
<p>BBZN-K ; E=-858.249648717H</p> 	<p>16  C,0.5634735902,-0.8937454097,-0.4274127276  C,0.5744516703,0.3476311755,-1.0603111089  C,-0.5877721219,1.1176153039,-1.2179214052  C,-1.822036408,0.6330157263,-0.759128725  C,-1.944374024,-0.595036458,-0.1122739829  H,-0.5415020876,2.0628552918,-1.7452583  B,-0.7367107316,-1.4984283514,0.0762347038  C,-0.8237590986,-2.9432489866,0.7547293896  H,-1.6357214285,-3.0297804058,1.4823708422  H,-1.0197311777,-3.7028143051,-0.0091912191  H,0.1039102144,-3.2438564521,1.2498688182  K,-0.239986018,0.9845477203,1.6755204166  H,1.5185960444,-1.4145015907,-0.370747735  H,1.5029738789,0.7481248537,-1.4623311905  H,-2.7019626634,1.2489139221,-0.9339678101  H,-2.9505455811,-0.8820684085,0.1908911202</p>
<p>BBZN-K:CO<sub>2</sub> ; E= -1046.85724750H</p>	<p>19  C,0.5656657884,-0.896477995,-0.4297854584  C,0.5774087384,0.345932052,-1.0618215989  C,-0.5819656338,1.1197700627,-1.2130000324  C,-1.8170562541,0.6339841912,-0.7567086222  C,-1.9405739841,-0.5942695012,-0.1119835228  H,-0.5345111747,2.0653530135,-1.7392593556  B,-0.7332988559,-1.4971243807,0.0803292285</p>

	<p>C,-0.8204161805,-2.9425485685,0.7563510842  H,-1.6333669786,-3.0301350697,1.4826010168  H,-1.0144921157,-3.7013573012,-0.0087708952  H,0.1063743217,-3.2429433458,1.253206701  K,-0.2850986758,1.0075242038,1.7079499367  C,3.1118794263,0.5131880214,0.8518997232  O,2.4574645049,0.9851693462,1.6883202814  O,3.7981313007,0.0666479365,0.0475917691  H,1.5132608964,-1.4348878328,-0.3977876459  H,1.5014420952,0.738982559,-1.484855482  H,-2.696601035,1.2500083578,-0.9327750993  H,-2.947466894,-0.8825868192,0.1873808317</p>
<p>BBZN-K/CO<sub>2</sub> (TS1) ; E=-1046.8292879H</p> 	<p>50  C,0.8945713286,0.9543138523,-1.2840941955  C,-0.4484090317,1.1725560436,-1.3464770527  C,-1.2871482027,1.2410252992,-0.1757876899  C,-0.6486149884,1.2792782916,1.1176376122  C,0.6866772196,1.0596683583,1.2931264419  H,-2.1940108171,1.822931895,-0.2765267315  C,3.1485167763,0.5761337726,0.2109317756  H,3.7023296819,1.5210268658,0.1758198329  H,3.4283260554,0.1083566637,1.1596023232  H,3.5538334142,-0.0234143181,-0.610710673  O,-3.3323256403,-0.2181627978,0.1487957033  C,-2.1704455411,-0.4070942759,-0.0447267822  O,-1.3938252967,-1.3424026852,-0.1660933388  B,1.5943008831,0.8996125788,0.0760436052  K,0.963586245,-1.9110356457,0.0859564707  H,1.4318055114,0.8800939367,-2.2281260499  H,-0.9513123468,1.265772435,-2.3059734417  H,-1.3044345215,1.4441486753,1.9692769646  H,1.0610712707,1.0612340548,2.3150182254</p>
<p>BBZN-K-CO<sub>2</sub> (int1) ; E=-1046.82989295H</p> 	<p>50  C,0.9909211229,-0.9417338895,1.292383257  C,-0.3522128918,-1.0910377448,1.3283178653  C,-1.2024169327,-1.1637845127,0.1331304855  C,-0.5069688815,-1.18732559,-1.1609053785  C,0.8290713823,-1.0148953649,-1.3043533499  H,-1.9423352252,-1.9597322321,0.2099091586  C,3.3009372917,-0.7948250102,-0.1557147862  H,3.7281733998,-1.7997926714,-0.0506143709  H,3.6607556424,-0.4111156897,-1.1124469519  H,3.7425852999,-0.2068836745,0.6532862673  O,-3.3038654031,-0.089641005,-0.4443498611  C,-2.2137351889,0.1648363005,0.0130408182  O,-1.6777216845,1.2344477544,0.3714611538  B,1.7299688422,-0.9316690801,-0.0615402819  K,0.6132714438,1.9399332432,0.077169833  H,1.5156368183,-0.8883138481,2.244413378  H,-0.8790050592,-1.1412899283,2.2782713435  H,-1.1567446565,-1.3065507502,-2.0246734328  H,1.2272906801,-1.0113093065,-2.316544147</p>
<p>BBZN-K/CO<sub>2</sub> (TS2) ; E=-1046.82726666H</p>	<p>50  C,1.2118047782,-0.6377777864,1.338829021  C,-0.1087226396,-0.8888151261,1.4430814177  C,-0.9921905442,-1.1598356975,0.2875747688  C,-0.3219742255,-1.2689180305,-1.0305335642  C,0.9885364492,-1.0167297099,-1.2315054911  H,-1.607978037,-2.0478662526,0.4682747277</p>

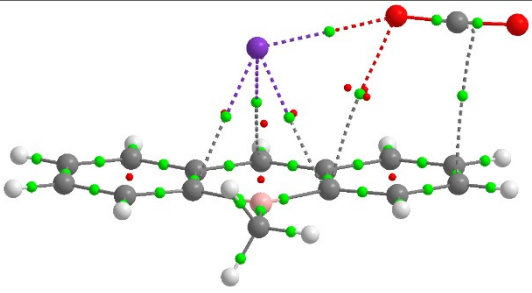
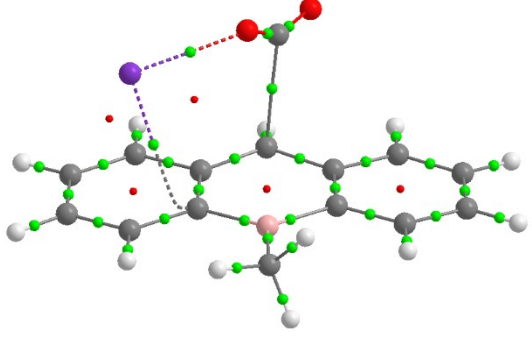
	<p>C,3.4627468583,-0.4790294725,-0.2031602986  H,3.9488823052,-1.457317893,-0.097014773  H,3.751316536,-0.1059257767,-1.1878346369  H,3.9026491207,0.1597167303,0.5650801061  O,-2.7587828299,-0.0186085567,-0.8988784609  C,-2.110821161,0.0116536911,0.1426462029  O,-2.0787049211,0.8763868264,1.0416007995  B,1.91393549,-0.705100053,-0.0335182491  K,-0.3074070036,1.932175808,-0.4474135333  H,1.7537344474,-0.4225011684,2.2566333921  H,-0.6124964059,-0.848128447,2.4034698265  H,-0.9893804195,-1.508424221,-1.8521161454  H,1.3613872024,-1.0955308646,-2.2503871098</p>
<p>BBZN-K-CO<sub>2</sub> (int2); E=-1046.84117651H</p> 	<p>50  C,2.1124399832,-0.0105554193,1.3113325941  C,0.953932599,-0.6803398788,1.2299158805  C,0.2901812733,-1.0264034575,-0.0590612248  C,0.9420718359,-0.5112034914,-1.2965305047  C,2.1001659174,0.1642346402,-1.2987447418  H,0.3136632432,-2.1280353727,-0.1328675543  C,4.1928869466,1.256017586,0.075436277  H,4.9927837533,0.5061591737,0.0212679848  H,4.345362243,1.9276685726,-0.7713235586  H,4.3538797354,1.8086194906,1.0028399104  O,-1.8156360978,-0.6007202202,-1.1363933138  C,-1.2402105053,-0.7562016123,-0.0337815064  O,-1.8052000623,-0.749653736,1.085064805  B,2.8191028658,0.4889967268,0.0305468326  K,-3.9725398758,-0.0436166718,0.0268455157  H,2.5111581741,0.1815956433,2.3046458251  H,0.418362481,-1.01469198,2.1121984638  H,0.3981553959,-0.7252615356,-2.2105220332  H,2.4897210939,0.4873705423,-2.2612396515</p>
<p>BBZN-K/CO<sub>2</sub> (TS3); E=-1046.83086579H</p> 	<p>50  C,1.9535447859,0.072908167,1.3022797737  C,1.4578641251,-1.1629008894,1.2558111891  C,0.7468324946,-1.6058958083,0.0000469309  C,1.4579834677,-1.1629585619,-1.2556698206  C,1.9536692142,0.0728480811,-1.3021483365  H,0.5153375479,-2.6668584743,0.0000604802  C,1.7196066809,2.5013720904,-0.000018773  H,2.7520664506,2.8717115515,0.0000353922  H,1.2369209545,2.9131583988,-0.8880807237  H,1.2368417619,2.9132006743,0.8880143696  O,-0.5104140897,0.4348278613,-0.0000601107  C,-0.6026158956,-0.8236169444,-0.0000318611  O,-1.6716330376,-1.4683903269,-0.0000572208  B,1.7577291895,0.9275682085,0.0000364576  K,-3.0041201065,0.6728260684,-0.0000949176  H,2.4053769018,0.4436798025,2.2176115342  H,1.4449105162,-1.8432320187,2.1012326283  H,1.4451089983,-1.8433281679,-2.1010614717  H,2.4055880404,0.4435772878,-2.217454416</p>
<p>BBZN-K-CO<sub>2</sub>; E=-1046.84324228H</p>	<p>50  C,-0.7033911157,1.2940755536,0.634268401  C,-0.8545156515,1.2578447659,-0.6847381131  C,-0.301381196,0.0007354645,-1.3668405331  C,-0.8602707367,-1.2538934584,-0.6848583536  C,-0.7091953416,-1.2910126989,0.634129934</p>

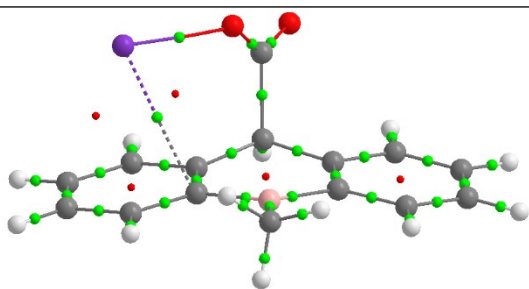
	<p>H,-0.4140830988,0.0010484846,-2.4463346427  C,0.6071344076,-0.0015327285,2.7228858055  H,-0.2387111119,0.0003281346,3.4159408168  H,1.2049005759,-0.8882095274,2.961059301  H,1.2088730589,0.8824274129,2.9611561804  O,1.4045050896,-0.0032058897,0.2716013405  C,1.1692691657,-0.0026322138,-1.0131667039  O,2.0919308425,-0.0046211516,-1.8299882063  B,0.0960508569,-0.0003028202,1.2046521466  K,3.8959053458,-0.0085797977,-0.0163477125  H,-1.0795931485,2.1289873852,1.2179690629  H,-1.3102928111,2.0186154135,-1.3078351291  H,-1.3195176257,-2.0125113366,-1.3080320585  H,-1.089130018,-2.1242970619,1.217738374</p>
<b>Boraanthracene<sup>(1)</sup></b>	
<p>BA ; E=-754.214965172H</p> 	<p>27  C,-7.7649041275,-1.8423791369,0.0144652364  C,-6.3922423863,-1.8721198062,0.0087315063  C,-5.5917462739,-0.7049306671,-0.0009737991  C,-6.2674792569,0.5630685782,-0.0048880834  C,-7.6969111733,0.5695521084,0.0012263397  C,-8.4201278068,-0.5884432022,0.0105516246  C,-5.5504044523,1.7671676184,-0.0144540654  C,-4.1511024127,1.810261312,-0.0207171879  C,-3.3601205443,0.6061026298,-0.0176436655  C,-1.9512965371,0.7561120965,-0.0245350083  H,-1.3411627055,-0.141392282,-0.0223450279  C,-1.3219009224,1.9753805291,-0.0338222529  C,-2.1096570634,3.1513380431,-0.0367496962  C,-3.4713135505,3.0691522985,-0.0304262948  H,-8.3428578865,-2.7589537013,0.0218662113  H,-5.8889790213,-2.8349902524,0.011730505  H,-8.2069913218,1.5282041169,-0.0017284021  H,-9.5045036719,-0.547687756,0.014995068  H,-6.1012906184,2.7031708775,-0.0171193873  H,-0.2405253532,2.0438584911,-0.0388619775  H,-1.6269964099,4.1232299304,-0.0440656914  H,-4.0700479423,3.9750366679,-0.0327172608  B,-4.0640600425,-0.7490608217,-0.0073166423  C,-3.2911777318,-2.1532004688,-0.0030721057  H,-2.2027911018,-2.0688395391,-0.0077367297  H,-3.5622959414,-2.7489979622,0.8753151502  H,-3.5690874943,-2.7579774915,-0.873165873</p>
<p>BA:CO<sub>2</sub> ; E=-754.214965172H</p> 	<p>30  C,-7.7690366602,-1.9982060189,-0.3281501568  C,-6.3967530103,-2.0121255084,-0.2937756141  C,-5.6088074785,-0.8382694929,-0.220508673  C,-6.3041671582,0.4215552784,-0.1867820065  C,-7.7341464634,0.4111264826,-0.2211899884  C,-8.4412179634,-0.7545447635,-0.2879228098  C,-5.6123113269,1.6385510375,-0.1022674444  C,-4.2117187379,1.7088042709,-0.0443727049  C,-3.4075971435,0.5204820796,-0.0672901429  C,-2.0038803279,0.6794635416,0.0050877101  H,-1.3877585524,-0.2150934651,-0.0095066704  C,-1.3907299769,1.9050664167,0.0937049257  C,-2.1925784651,3.069312846,0.1144963523  C,-3.5533540847,2.9734790716,0.0473723947</p>

	<p>H,-8.3338270997,-2.9212550626,-0.3821657783  H,-5.8876454358,-2.9699852447,-0.3206890911  H,-8.2549317687,1.3629659554,-0.1842604657  H,-9.5256928034,-0.7271733281,-0.309902035  H,-6.1832046453,2.5620992521,-0.0867807129  H,-0.3115940474,1.9861068667,0.1481270564  H,-1.7230328347,4.045063578,0.18400165  H,-4.1633716995,3.8716857038,0.0633746992  B,-4.0816993904,-0.849245814,-0.1596591607  C,-3.2016911072,-2.1868318736,-0.1812240219  H,-2.4794509254,-2.1703307452,-1.0044280286  H,-2.6108786212,-2.2776260015,0.7367343197  H,-3.7810572559,-3.1063979014,-0.2813060588  C,-6.1265081093,1.2728711856,2.7800344853  O,-6.9728222895,2.063877989,2.7375115169  O,-5.2967131974,0.4844589847,2.9205076741</p>
<p>BA/CO<sub>2</sub>; E=-754.203178385H</p> 	<p>30  C,3.7072034156,0.8076938761,-0.7219274484  C,2.556032724,1.4674182753,-0.351346431  C,1.3037644231,0.8262548477,-0.2881871219  C,1.2471804803,-0.5557246951,-0.608854402  C,2.4378537413,-1.2249326797,-0.9739665261  C,3.6372094243,-0.5588356953,-1.0344648948  C,0.0159245365,-1.2898482331,-0.5018557459  C,-1.2454290457,-0.6001001294,-0.4754719522  C,-1.3108017751,0.7777230031,-0.1483956324  C,-2.5805617577,1.3800413692,-0.0670541415  H,-2.6393199435,2.4331519964,0.1904984682  C,-3.7446710428,0.6835717271,-0.3082060859  C,-3.6660762572,-0.6796070363,-0.6333709801  C,-2.4466718508,-1.3074550897,-0.709325562  H,4.6552198557,1.3299208985,-0.7675851387  H,2.6127175909,2.5227671421,-0.1064952196  H,2.3890362201,-2.2840916838,-1.2028619277  H,4.535703212,-1.0928755526,-1.3237039696  H,0.0102649169,-2.2774645757,-0.9476439276  H,-4.7083980421,1.1743083915,-0.2446880581  H,-4.5738025542,-1.2418591247,-0.8231913582  H,-2.3903455943,-2.3645603593,-0.9461209066  C,-0.036568186,3.0611950664,0.5977167463  H,-0.7111697259,3.1641558345,1.4521144792  H,0.9354988047,3.4562321822,0.8953663381  H,-0.4313760683,3.7202619282,-0.1840415192  O,0.145118481,-0.9258869866,2.1231636445  C,0.1337747137,-1.8898962288,1.4235123811  O,0.1634227957,-3.0877372306,1.3829277029  B,-0.0007184918,1.5564207622,0.0845231898</p>
<p>BA-CO<sub>2</sub>; E=-754.248842540H</p>	<p>30  C,-7.5308129562,-1.5130661252,-1.0252077003  C,-6.2432681678,-1.7190950645,-0.5277519711  C,-5.5793109219,-0.7217012342,0.1723120408  C,-6.2421136223,0.4999417655,0.3600095289  C,-7.5234872254,0.7158153594,-0.1171491877  C,-8.171109327,-0.299750683,-0.8191692454  C,-5.4259533131,1.5311155949,1.1197498205  C,-4.1201654898,1.7460262942,0.3745136448  C,-3.3742995065,0.5731723496,0.187303542  C,-2.1727947941,0.6712547523,-0.5000771557  H,-1.5723418797,-0.2198418029,-0.6573954362</p>

	<p>C,-1.720500516,1.8989865188,-0.9856517648  C,-2.470241742,3.0480224501,-0.7802942553  C,-3.6796733984,2.9730423689,-0.0908935798  H,-8.036662482,-2.3025823209,-1.5699404448  H,-5.7559871941,-2.6766541372,-0.6858162113  H,-8.0178593763,1.6671345954,0.0500434211  H,-9.1724778253,-0.140183076,-1.201701902  H,-5.9696855775,2.4548537732,1.3060542221  H,-0.7791205303,1.9593527683,-1.520547171  H,-2.1179400512,4.0025212503,-1.1535872565  H,-4.2713155641,3.8672367836,0.0756645457  C,-3.2936730933,-2.0972772419,0.8953291972  H,-3.078049817,-2.452809722,-0.1184738395  H,-2.3356577131,-1.9929895628,1.4140537515  H,-3.856644391,-2.8861305589,1.4037762252  O,-4.3924410649,-0.2425585533,2.3185207281  C,-5.0498281364,0.8747788322,2.4622571371  O,-5.3470057999,1.3693539219,3.5288644364  B,-4.1058248734,-0.7139136757,0.8656266301</p>
<b>Boraanthracene<sup>(-):K<sup>(+)</sup></sup></b>	
<p>BA-K ; E=-1165.52440662H</p> 	<p>28  C,-3.7337912098,0.368986769,0.0973233038  C,-2.5785984746,1.1014798122,0.0529792868  C,-1.2899599213,0.5050156801,-0.0192712113  C,-1.2259021269,-0.9305974934,-0.0531247041  C,-2.4483230713,-1.6716924529,-0.0148016712  C,-3.6571790688,-1.0441783851,0.0598772334  C,0.0122231541,-1.6000413409,-0.0722980389  C,1.2411462752,-0.9162545295,-0.054964124  C,1.2966401943,0.5234371918,-0.0199879037  C,2.5856181087,1.1219425278,0.0570228946  H,2.6476903795,2.2038894932,0.0753396049  C,3.743193511,0.3946958278,0.102534733  C,3.674003627,-1.0191040424,0.0601454454  C,2.4686615769,-1.6508604075,-0.0179823251  H,-4.6986013276,0.8568198822,0.1470548411  H,-2.6393275173,2.1847760083,0.0658343033  H,-2.3979302802,-2.7546467812,-0.0544155137  H,-4.567919369,-1.6307617281,0.0823360317  H,0.0191800478,-2.6840260437,-0.1227334393  H,4.7051532045,0.8876001804,0.1563477722  H,4.587400617,-1.6015795066,0.0819932614  H,2.4226239175,-2.733870548,-0.0604602048  B,-0.0018836064,1.3328160137,-0.0673540949  C,-0.0573872362,2.9258441091,-0.0852242175  H,0.9170072008,3.4131586949,-0.1229979034  H,-0.6214462812,3.2754872372,-0.9553818368  H,-0.584497605,3.3302166037,0.7860046198  K,0.0094048815,-0.3052275922,2.5044977375</p>
<p>BA-K:CO<sub>2</sub> ; E=-1354.13513647H</p>	<p>31  C,-3.4277192534,-1.2407742052,0.7173370471  C,-2.2025332916,-1.3358118049,1.319866413  C,-1.020054655,-0.7713447992,0.766607392  C,-1.1470905598,-0.0816072914,-0.4922969838  C,-2.4410362821,0.0057751559,-1.0998295573  C,-3.5408399626,-0.5467626039,-0.5150279907  C,-0.0304392091,0.4748842686,-1.136961597  C,1.2676103922,0.4071888378,-0.5941408579</p>

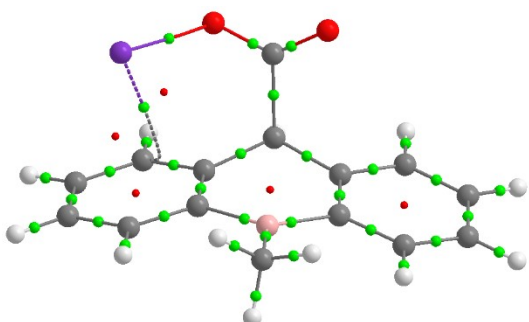


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<p>BA-K/CO<sub>2</sub> (TS1); E=-1354.11841913H</p> 	<p>31  C,-3.9405579536,-0.011709673,0.674034719  C,-2.9323298224,-0.9487210812,0.5787542253  C,-1.6464742743,-0.6444051609,0.0754196056  C,-1.4123224174,0.6861390413,-0.4033909198  C,-2.4645523439,1.6401419917,-0.2922747754  C,-3.6887362876,1.3051955878,0.2304246773  C,-0.1544861421,1.0737537283,-0.9269829974  C,0.8738633889,0.1071653595,-1.1916236891  C,0.7641494742,-1.2298215956,-0.7240206603  C,1.838925597,-2.1106613458,-0.9798088616  H,1.766162121,-3.1337135686,-0.6272297464  C,2.9603992658,-1.7183501895,-1.6675741528  C,3.05003661,-0.3950588861,-2.1334268667  C,2.035473201,0.49638593,-1.9009309986  H,-4.9205891883,-0.2843503035,1.0440424659  H,-3.1335075293,-1.9648653747,0.8999505769  H,-2.2883694,2.6487373919,-0.6509700982  H,-4.474893862,2.0494790028,0.279668593  H,-0.1145396943,2.0088101205,-1.4726806788  H,3.766811343,-2.4153481868,-1.8553978533  H,3.9290217339,-0.0770038773,-2.6810406262  H,2.1152520966,1.5183569474,-2.2519586246  C,-0.6575251487,-3.169127838,0.5436763787  H,-1.5397344193,-3.3505633482,1.1592465685  H,-0.6997810467,-3.8811628521,-0.2871674342  H,0.2174746889,-3.4546647386,1.1338464182  O,1.5980978067,2.8015485295,0.2287125167  C,0.9174038017,2.0121018833,0.7618432367  O,0.5048925378,1.4764056615,1.7457513544  B,-0.5146856731,-1.6917008736,-0.0183452782  K,-1.7464524636,0.7914087179,2.6407919255</p>
<p>BA-K-CO<sub>2</sub> (inte1); E=-1354.13236177H</p>	<p>31  C,-3.2435889395,-1.1284997345,-1.0697393266  C,-2.1328646465,-1.7376826241,-0.5070574316  C,-0.8894013694,-1.0873727728,-0.4286582711</p>

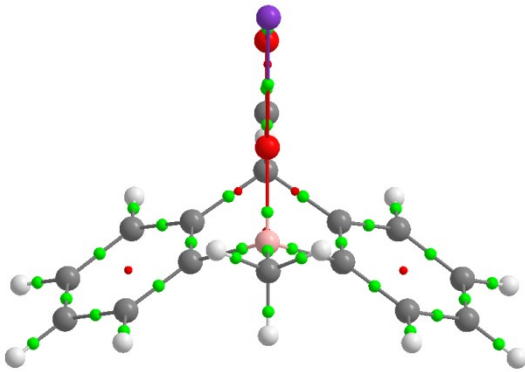
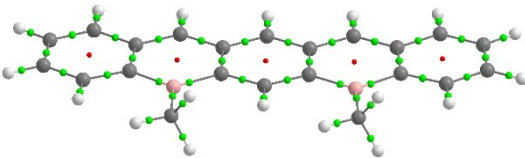


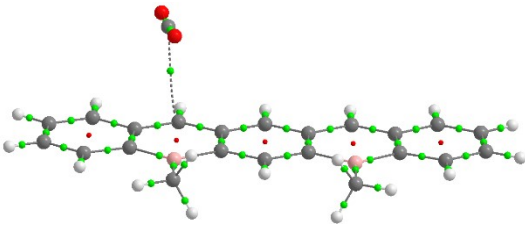
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 H,2.9600965451,-2.6764976921,0.6371336649  
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 C,4.1367669404,0.2947546865,-0.4431314902  
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 H,-4.1874698829,-1.6548505588,-1.1359646639  
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 H,-1.8137568801,1.831633313,-1.9119085757  
 H,-3.9744024272,0.6480852685,-2.043697925  
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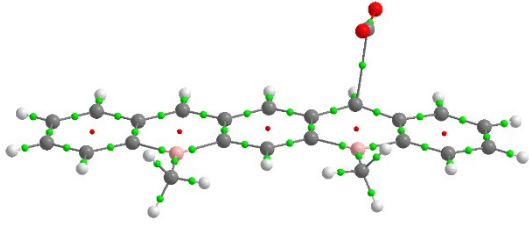
BA-K/CO<sub>2</sub> (TS2); E=-1354.12693131H

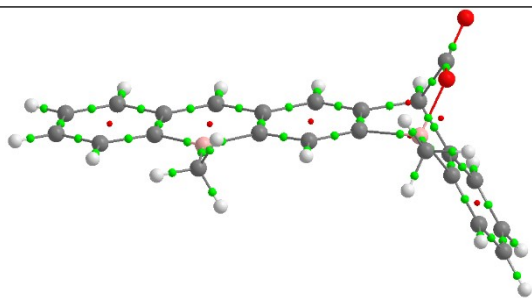


31  
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 C,2.0667325656,1.7558004303,-0.4963372374  
 C,0.8538734142,1.0589461098,-0.3672798117  
 C,0.7732051296,-0.2499482099,-0.8803705596  
 C,1.8771072962,-0.7992437157,-1.543256297  
 C,3.0555792155,-0.0831378892,-1.6770499292  
 C,-0.4233509713,-1.1008466591,-0.6106584561  
 C,-1.7171783314,-0.3649970508,-0.4565481255  
 C,-1.7546890366,0.973038337,-0.0260452492  
 C,-3.0060132544,1.5816714791,0.1592291984  
 H,-3.0483808001,2.6128207443,0.4906702579  
 C,-4.1834085726,0.9014496256,-0.0801430872  
 C,-4.1277212739,-0.4279804303,-0.4916411998  
 C,-2.9077796909,-1.054666412,-0.6683530494  
 H,4.0827731593,1.7626066377,-1.2440914088  
 H,2.1362076668,2.7663057131,-0.1089414949  
 H,1.8058066111,-1.8060472344,-1.9344168128  
 H,3.8931798137,-0.518481488,-2.2088573786  
 H,-0.5153082341,-1.8584956143,-1.3924782439  
 H,-5.139358446,1.3893624371,0.0591660983  
 H,-5.0441035273,-0.9774462389,-0.6681944867  
 H,-2.8721325765,-2.0965844147,-0.9627423146  
 C,-0.3643845986,3.1451119936,0.90858877  
 H,-0.3704098602,3.9160745558,0.1278140086  
 H,-1.2111582308,3.3524357849,1.5619648522  
 H,0.5524838135,3.3017602335,1.4807496629  
 O,-0.9991214281,-2.0664257172,1.5450506164  
 C,-0.1052247077,-1.9692685852,0.7243255696  
 O,1.0665659382,-2.4330016748,0.7542594102  
 B,-0.4345886059,1.7330512874,0.2166157547

<p>BA-K-CO<sub>2</sub>; E=-1354.15862490H</p> 	<p>K,2.7617504428,-0.8003941053,1.3863305909 31 C,3.3887687663,0.6776161531,-1.2941820719 C,2.3726854787,1.3505204854,-0.6171035249 C,1.284388667,0.660100597,-0.1025403877 C,1.2402280192,-0.7273558999,-0.2871902919 C,2.2465509645,-1.4122093799,-0.9450936374 C,3.3276581332,-0.6985389455,-1.4567918385 C,-0.0001721088,-1.3964343487,0.2948714679 C,-1.2403144697,-0.7272558603,-0.2874829833 C,-1.2845134232,0.6601917156,-0.1027220364 C,-2.372767359,1.3506309364,-0.6173150052 H,-2.4349075351,2.4268090488,-0.4925704209 C,-3.3887592686,0.6777932139,-1.2945736505 C,-3.3276125684,-0.6983392663,-1.4573196393 C,-2.2465430556,-1.4120432582,-0.9455795562 H,4.2309777537,1.2286540411,-1.694788184 H,2.4347997361,2.4267105057,-0.4924514649 H,2.1913846467,-2.4878203119,-1.0701096421 H,4.1173925806,-1.2193305499,-1.9834150734 H,-0.0001639006,-2.4776512831,0.1812198743 H,-4.230917582,1.2288753651,-1.695223148 H,-4.1172914434,-1.2190916616,-1.9840614617 H,-2.191389045,-2.487652221,-1.0706239127 C,-0.0000211491,2.7222093855,1.2311672464 H,0.0001743194,3.4222361895,0.390752144 H,-0.8858068133,2.9557592913,1.8316234277 H,0.8857045625,2.9555186048,1.8318111173 O,-0.0003855294,0.2514658151,2.0004178281 C,-0.000159512,-1.0347135166,1.7661125003 O,0.0004524373,-1.8488841112,2.6862973145 B,-0.0001058061,1.2098976367,0.712504303 K,-0.000172036,-0.0377639007,4.5065689971</p>
<b><u>cis-Diborapentacene<sup>(2-)</sup></u></b>	
<p>cis-DBP; E=-898.897611336H</p> 	<p>42 C,2.5687288222,1.1611108916,-0.0001177127 C,1.3126139619,0.545511622,-0.0000900049 C,1.292505319,-0.9011810296,-0.0000905188 C,0.0500065142,-1.5907760019,-0.0000621708 C,-1.1803550997,-0.9479194586,-0.0000167279 C,-1.2910809215,0.5002765837,-0.0000159025 C,-2.5881394025,1.0549205858,0.0000510028 H,-2.6776024361,2.137995477,0.0000438431 C,-3.7450132336,0.3056597057,0.0001063912 C,-3.628720257,-1.1076400266,0.0001078971 C,-2.4031510274,-1.7059975814,0.0000515112 H,2.5844518953,2.2484655706,-0.0001164822 H,0.0678596201,-2.6780786713,-0.0000555121 H,-4.7208447346,0.7781355412,0.0001526206 H,-4.5258567386,-1.721407119,0.0001581441 H,-2.3297743203,-2.7904338623,0.0000605709 B,-0.005762932,1.3291624684,-0.0001134263 C,0.0039627406,2.9352952641,0.0000059634 H,-0.9885224664,3.3925945232,0.000385964 H,0.5413416677,3.3208367321,0.8732997866 H,0.5407027553,3.3209206648,-0.8736466408 C,4.9662884777,-1.7028452285,-0.0000393907 H,4.893575097,-2.7877916157,0.0000581562</p>

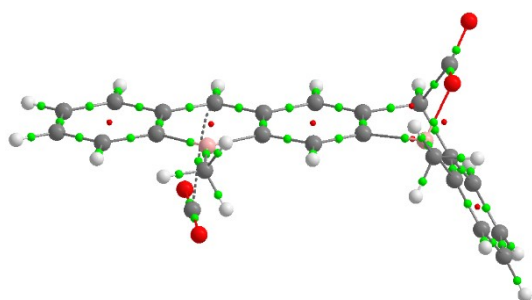
	<p>C,6.2277119613,-1.1209409065,-0.0000562525  C,6.400308352,0.3175305588,-0.0000674588  C,7.7159095217,0.8221480765,0.0000646089  H,7.8426876597,1.9027953555,0.0000231669  C,8.8419416689,0.0258242043,0.0001709311  H,9.8368977631,0.4566001874,0.0002325058  C,8.6664614244,-1.3806374896,0.0001587985  H,9.5373731564,-2.0310215965,0.0002179306  C,7.4166033294,-1.9291749119,0.0000765151  H,7.299655694,-3.0098212145,0.0001164272  C,3.7601766884,-0.9528542646,-0.000104911  C,2.5114562508,-1.5913115377,-0.0001018116  H,2.4891493902,-2.679823409,-0.0000831192  C,3.8027634157,0.4969749188,-0.0001344778  C,5.3158364821,2.8107886931,-0.0000288613  H,5.8808427257,3.1491194105,0.8763085581  H,5.8844229464,3.1490715464,-0.8740489944  H,4.3671560822,3.3502808878,-0.0019521329  B,5.1585371461,1.2114032962,-0.0001346242</p>
<p>cis-DBP:CO<sub>2</sub> ; E=-1087.50626671H</p> 	<p>45  C,0.1357192003,1.315037517,-0.0524521933  C,1.3219351691,0.5650620561,-0.0383318691  C,1.2320717521,-0.8779253283,0.0006458928  C,3.8337842491,-0.9571175589,-0.015069258  C,3.7930540412,0.4933623477,-0.0530840594  C,5.0496953096,1.1920683703,-0.0808018579  H,5.0279955614,2.2783082338,-0.1090788811  C,6.2454045418,0.5359863952,-0.0724915704  C,6.2936045208,-0.8806887522,-0.0356298418  C,5.103165323,-1.573610129,-0.0083472911  H,0.2095938044,2.4007559075,-0.0840434929  H,7.1708091418,1.1055710363,-0.0944192508  H,7.2457704697,-1.3991480084,-0.0289137802  H,5.1407508989,-2.6592249033,0.0199747596  C,-3.84124479,-0.4253993324,0.0192846499  C,-3.6028340215,1.0042522477,-0.0258462207  C,-4.7503295196,1.8706167131,-0.0271600253  H,-4.5791586019,2.9432920311,-0.0523605403  C,-6.0249485908,1.3833370906,0.0111784155  H,-6.8632463236,2.0749082638,0.0110488977  C,-6.2661700061,-0.0116020213,0.0507845021  H,-7.2799181339,-0.3945963615,0.0801347587  C,-5.1810021574,-0.8622255248,0.0541818418  H,-5.366366276,-1.9322286027,0.0882213408  C,-1.2495399249,-0.7066873697,0.0073720813  C,-0.0532366454,-1.4321938768,0.0227322054  H,-0.1278898968,-2.517893449,0.0549574776  C,-1.1384781869,0.7340186602,-0.03440573  C,-2.7692025894,-2.9642949329,0.0958675089  H,-2.2920774271,-3.3585689662,0.9995966011  H,-3.7980906922,-3.3316987895,0.0839771285  H,-2.2453397466,-3.4303459316,-0.7454065837  B,-2.6333951787,-1.3665429748,0.0393791171  C,-2.3160893091,1.5337554833,-0.0476900758  H,-2.2010207547,2.6137782331,-0.0889371623  C,-2.6405446735,1.7143355881,2.8178039922  O,-2.5374431042,0.5818091791,3.0085457736  O,-2.7561776162,2.8681058416,2.7597143138  C,2.4245435058,-3.326711861,0.0575349588</p>

	<p>H,1.8712886253,-3.662778031,0.9411484141  H,1.8678021754,-3.7089661205,-0.8049662317  H,3.3937221784,-3.8312764049,0.0688472936  C,2.5940058065,1.1946333258,-0.0631448606  H,2.6278694187,2.2810219787,-0.0922364596  B,2.5112891736,-1.7238253495,0.014854411</p>
<p>cis-DBP/CO<sub>2</sub> (TS1); E=-1087.50197253H</p> 	<p>45  C,3.7771393821,1.0234513963,-0.3113353003  C,2.5442380134,1.5936836132,0.0356503503  C,1.3033870251,0.9588456062,-0.0574265932  C,1.3006170479,-0.4033760657,-0.5371919815  C,2.5075679491,-1.0030547502,-0.8789328072  C,3.7500041998,-0.3417392716,-0.792183096  C,0.0602902793,-1.1237454694,-0.6433145529  C,-1.1984393097,-0.4897721667,-0.5314259933  C,-1.3127620698,0.8534803449,-0.0446377756  C,-2.6004931046,1.3979766474,0.0981574024  H,-2.6866623694,2.4147720039,0.4731937207  C,-3.7535856199,0.707132139,-0.2203851987  C,-3.6312528999,-0.6082580963,-0.7085437234  C,-2.398290947,-1.187918348,-0.8594981278  H,2.5542365002,2.618111797,0.395415509  H,2.4946286383,-2.0295768847,-1.2395243526  H,0.0912821862,-2.0899569384,-1.1346704072  H,-4.7305461583,1.1617886614,-0.1018293412  H,-4.522923893,-1.1712039412,-0.9692740845  H,-2.3164217943,-2.2065333242,-1.2258899213  C,-0.1329777493,3.1180662368,0.8818184938  H,-0.7502680649,3.1174333623,1.7866818737  H,0.8280269767,3.5651047505,1.1394297021  H,-0.6305819531,3.7927214816,0.1754663184  O,0.0307464975,-1.2082713031,2.1768461879  C,-0.13269359,-2.0859761239,1.4135534278  O,-0.3452945992,-3.2128816346,1.1177608845  B,-0.0255263568,1.6410143744,0.2761269501  C,4.9467314919,-0.9910293796,-1.1711314691  C,6.3545987758,0.9808867166,-0.6539491236  C,6.1977841364,-0.379824807,-1.1145097514  C,7.6563099423,1.5223419803,-0.6324233693  C,7.3809859916,-1.0855518166,-1.5154459189  C,8.7786975084,0.8254786845,-1.0245652289  H,9.7626121275,1.2796981366,-0.9920801467  C,8.6179522588,-0.508185524,-1.4729016531  H,9.4879804155,-1.0787797472,-1.7863253706  H,4.8849099486,-2.0170538613,-1.5243903846  H,7.2730361716,-2.1100097528,-1.8613693549  H,7.7731457042,2.5468057733,-0.2860813358  B,5.1141915454,1.7637644654,-0.2164031702  C,5.2568673888,3.27714637,0.3013126078  H,4.313947768,3.7348216007,0.6054783318  H,5.9376392777,3.3357102311,1.158161879  H,5.6927410712,3.9167737232,-0.4748749656</p>
<p>cis-DBP-CO<sub>2</sub> ; E=-1087.54944107H</p>	<p>45  C,0.1517091999,-0.9548204474,0.6616486013  C,1.3015124995,-0.5283423196,0.0651819077  C,1.3468528826,0.6323327052,-0.7579636574  C,3.7802914524,0.9403964508,-0.0116368795  C,3.6399155912,-0.2179493619,0.772016429  C,4.352133729,-0.3920110648,1.9465062954</p>

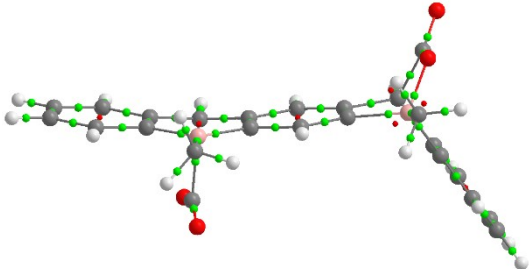


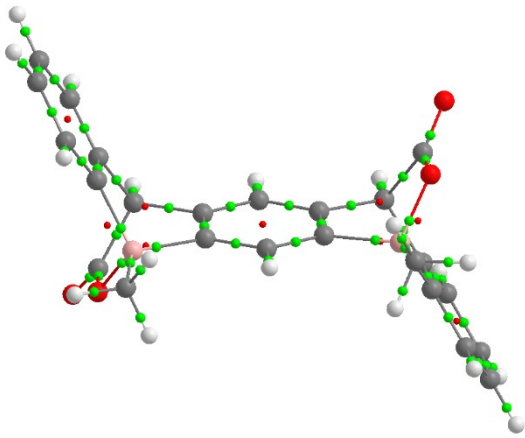
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 C,5.3720694415,1.7635915624,1.6250598309  
 C,4.653895708,1.921502484,0.4377766445  
 H,0.1501483496,-1.8504492222,1.2794490049  
 H,5.7798394013,0.4824635917,3.3012577881  
 H,6.0486296923,2.5429461358,1.9612817686  
 H,4.781840791,2.8287046995,-0.1465385969  
 C,-3.5965789834,1.1818079787,0.2056891211  
 C,-3.4706882439,-0.0213621581,1.0004710407  
 C,-4.6417103536,-0.5195999113,1.6622440281  
 H,-4.545171265,-1.4233725833,2.2582367036  
 C,-5.8506581753,0.1038516024,1.561403364  
 H,-6.7147679783,-0.3049924084,2.0775817278  
 C,-5.9860814438,1.2834781267,0.785615974  
 H,-6.9475701801,1.7787824446,0.7059126096  
 C,-4.8774031008,1.7803257763,0.1417304533  
 H,-4.9879048635,2.6839295392,-0.451031456  
 C,-1.0639363534,0.9449022387,-0.3201498298  
 C,0.1733280046,1.3249725138,-0.9201701046  
 H,0.1778644751,2.216710126,-1.5452382142  
 C,-1.070734038,-0.2331050841,0.4931719646  
 C,-2.3851544855,3.0565651766,-1.415785671  
 H,-3.3617912126,3.542995437,-1.4812164636  
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 H,-2.063284468,2.8347544771,-2.4392012526  
 B,-2.3610578464,1.7300489451,-0.5086981306  
 C,-2.2512968254,-0.6822777891,1.1235787996  
 H,-2.2039201648,-1.5830575067,1.7304055372  
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 H,4.0860297273,2.0881266818,-2.7863654316  
 C,2.6498959244,-1.2221226263,0.211522851  
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 B,2.8380816948,0.8771544135,-1.3427616179  
 C,3.1429021146,-1.547794558,-1.2085272714  
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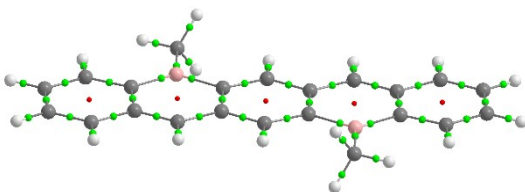


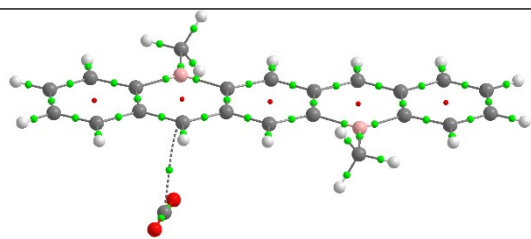
48  
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 C,3.4610202769,-0.7814007442,0.0732265832  
 C,4.0112657792,-2.0128740848,0.3856729523  
 H,3.8965290042,-2.850019932,-0.2957653731  
 C,4.7043538593,-2.1729383799,1.5858153319  
 C,4.8395247868,-1.0966783192,2.4507750438  
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 H,0.1224966285,-1.4450544164,-1.8057536685  
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 H,5.3770729163,-1.2206238744,3.3854999222  
 H,4.4023115159,0.9786673864,2.8016900123  
 C,-3.7279009599,0.9606694006,0.138969987  
 C,-3.5945481779,-0.1974857317,-0.7162772998  
 C,-4.7889672472,-0.8732320813,-1.1330096535  
 H,-4.6854386557,-1.7487753601,-1.7679078761  
 C,-6.0281340316,-0.4528642094,-0.744447349

	<p>H,-6.9099498597,-0.9924203751,-1.077801542  C,-6.1712476341,0.6831829494,0.0900690949  H,-7.1565225621,1.0162915538,0.3967283704  C,-5.0388466493,1.3469563698,0.501467309  H,-5.1547728654,2.2151177853,1.143619901  C,-1.1318592536,1.1110684925,0.1259764718  C,0.1314845672,1.6723117191,0.4756886282  H,0.1326555231,2.5546541457,1.1136408735  C,-1.1323622329,-0.04225549,-0.7192802086  C,-2.4948572334,2.9760735445,1.5614699626  H,-1.9899936717,3.8232338136,1.084779175  H,-3.4968462496,3.3104567208,1.8414396068  H,-1.944448041,2.7851157078,2.4890788373  B,-2.4641774486,1.6840518882,0.6091781452  C,-2.3403817259,-0.6630262878,-1.1130918592  H,-2.2885036139,-1.5310228591,-1.7649190374  C,-2.8371688263,-2.5099433791,1.1127700738  O,-2.6449713597,-1.7322782413,1.9416180311  O,-3.0439382912,-3.3750089336,0.3671190405  C,3.1033935829,3.0375494332,1.0827098295  H,2.6180627682,3.8696408329,0.5633470281  H,2.6874260582,3.0025017323,2.095780149  H,4.1691632604,3.2772352372,1.1712400997  C,2.6711226949,-0.4902304733,-1.1892686802  H,2.6291091055,-1.3387474894,-1.869698463  B,2.8617444849,1.6467769534,0.3123860313  C,3.3934548165,0.6830281923,-1.8736573669  O,3.4877757045,1.7408836983,-1.1208172956  O,3.8383587513,0.6018009828,-3.0041457996</p>
<p>cis-DBP-CO<sub>2</sub>/CO<sub>2</sub> ; E=-1276.15012458H</p> 	<p>48  C,-0.0700067417,0.8170827539,-0.8861964282  C,-1.2386151311,0.1289841664,-0.6916275247  C,-1.273958735,-1.1372227785,-0.0585822256  C,-3.6404128524,-0.5622930141,0.7463447024  C,-3.512614869,0.6722353965,0.088717342  C,-4.1656505015,1.8072120129,0.5379192822  H,-4.0499374032,2.7484897917,0.0102255431  C,-4.9631009984,1.73462454,1.68001549  C,-5.0978850329,0.5273629398,2.3500322722  C,-4.4398038193,-0.6108521154,1.8801972856  H,-0.0746941634,1.7863128076,-1.3785629243  H,-5.4709865162,2.6208699268,2.044062585  H,-5.7160451582,0.4713945304,3.2402528085  H,-4.5560009104,-1.5520102265,2.4105372308  C,3.7874438424,-0.844586277,0.1709421662  C,3.657230731,0.4096358826,-0.4940255489  C,4.8322877633,1.0667022234,-0.9475508525  H,4.7276570909,2.0257349939,-1.444668633  C,6.0751816015,0.519648116,-0.7557787197  H,6.9550477784,1.0433864483,-1.1164672924  C,6.2176177208,-0.7143118626,-0.0936727542  H,7.2015757459,-1.1433149651,0.0587998206  C,5.0850942877,-1.3604212931,0.3542935477  H,5.1915418247,-2.313255293,0.8656178461  C,1.1710733165,-0.9899177008,0.1983985515  C,-0.0747400421,-1.651121395,0.3753945734  H,-0.074548422,-2.6230678919,0.8630998975  C,1.1653864167,0.272804804,-0.4523824157  C,2.6446304111,-2.9515537547,1.451011622</p>

	<p>H,1.6993382324,-3.3080048579,1.8616679283  H,3.0437527863,-3.7486656117,0.8125378366  H,3.3491018783,-2.8440659373,2.2820040857  B,2.5153731939,-1.5873734775,0.6290258374  C,2.3787845793,1.0169404667,-0.6537307891  H,2.3207263676,1.8722698775,-1.3169061192  C,2.5327246772,2.2182335856,1.1118374262  O,2.4292751368,1.4929743526,2.0399092493  O,2.691288171,3.3208490543,0.6841388246  C,-2.9901336138,-3.2359267944,0.5133396469  H,-2.4134110715,-3.9469997976,-0.08629975  H,-2.6570269649,-3.3430646057,1.5516880107  H,-4.0413419772,-3.5423001531,0.4710677432  H,-2.5646432036,1.5779322292,-1.6614446176  B,-2.7835675489,-1.7282012444,-0.0052542251  C,-3.2005159479,-0.452025777,-2.0506140708  O,-3.2861208113,-1.6213200658,-1.4838607299  O,-3.5597381941,-0.2110925213,-3.1879797954  C,-2.6077752737,0.6295314415,-1.1296154696</p>
<p>cis-DBP-(CO<sub>2</sub>)<sub>2</sub> ; E=-1276.19485245H</p> 	<p>48  C,0.0458519072,0.7440421383,-1.2813922955  C,-1.1156232883,0.107422702,-0.8616714121  C,-1.1748099604,-0.5992640743,0.3435713869  C,-3.6696707197,0.0007879453,0.4596396869  C,-3.5123957801,0.6868909656,-0.7558464447  C,-4.296986415,1.7799062308,-1.0806757813  H,-4.1578941404,2.2894690511,-2.0289738405  C,-5.25884369,2.229495219,-0.175275751  C,-5.4253743269,1.5723550538,1.0347986756  C,-4.6347353931,0.4628721025,1.3431773934  H,0.0743389131,1.2827304104,-2.2254991749  H,-5.8701869881,3.0920629678,-0.4168547798  H,-6.171768332,1.9230183957,1.7402669671  H,-4.7787472774,-0.0484706584,2.291012945  C,3.6576719787,-0.4718582092,0.4111466201  C,3.5737275867,0.2283511103,-0.8035808903  C,4.4002807496,-0.0692716143,-1.8731351625  H,4.3177128254,0.4905502767,-2.7994406887  C,5.3312182154,-1.1021122535,-1.7562801384  H,5.9750237453,-1.3495426561,-2.5931900088  C,5.4254158376,-1.8126895738,-0.568830037  H,6.1478031853,-2.6174952501,-0.4782667108  C,4.5931350578,-1.4923497709,0.5062725362  H,4.6805081374,-2.0510560744,1.4340693899  C,1.1560910613,-0.0017415154,0.7548142635  C,-0.0271112723,-0.6359790229,1.1371786174  H,-0.0556305354,-1.1753096779,2.0824879337  C,1.1701394061,0.6768653589,-0.4678100163  C,2.7123201878,-0.4555296856,3.005702764  H,2.5062764574,-1.5311270747,3.0390619691  H,3.7130888359,-0.2979778584,3.4233062802  H,1.9942730798,0.0313957999,3.6727230675  B,2.5940464276,0.1077483778,1.5046766437  C,2.5111916882,1.3128160699,-0.8111081846  H,2.4905540239,1.8806850864,-1.7395149943  C,2.8696517144,2.2482434298,0.3560638381  O,2.9106602094,1.6393441553,1.5065643345  O,3.103428473,3.431836057,0.1953293318  C,-2.8433298665,-2.2644944759,1.8058408624</p>

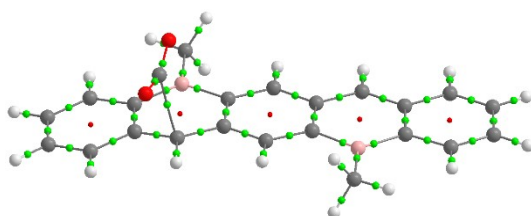


	<p>H,-2.1439977801,-3.1049019793,1.7582235155  H,-2.6669781533,-1.7510339603,2.7575422755  H,-3.8576626652,-2.6779362822,1.8367994743  H,-2.3451031534,0.6226612956,-2.6031497433  C,-2.4226641796,0.1137699521,-1.6441061452  B,-2.6422278538,-1.2628284263,0.5645383109  O,-2.9180095582,-2.036053808,-0.7662657703  C,-2.809082394,-1.3574763843,-1.8726403688  O,-3.0042510008,-1.8158568855,-2.983031634</p>
<b><u>trans-Diborapentacene<sup>(2-)</sup></u></b>	
<p>trans-DBP; E=-898.893911750H</p> 	<p>42  C,0.0260717315,1.3765037499,-0.0002654905  C,1.2474440053,0.7004678956,0.0035925215  C,1.2128878538,-0.7413166042,0.0070604496  C,2.4216956531,-1.4938662785,0.0111069938  C,3.6758716998,-0.9107364794,0.011973674  C,3.8461371799,0.5358900998,0.0087400768  C,5.1738727034,1.0299550763,0.0099757038  H,5.3133670473,2.1077616497,0.0075959089  C,6.2906708549,0.2302423708,0.0139977116  C,6.1136448055,-1.1829005832,0.0171291849  C,4.8651015945,-1.7238672273,0.0161498432  H,0.0360135732,2.4653837126,-0.0029040968  H,2.3478294307,-2.5787987552,0.0136326955  H,7.2872169139,0.6577815007,0.0147825005  H,6.9836837684,-1.8341319512,0.0203249377  H,4.7416414572,-2.8039184295,0.0185674077  B,2.6122582175,1.4219483163,0.0042947511  C,2.6674965395,3.026851099,0.0005054346  H,3.6772927975,3.4447367911,0.0010999261  H,2.1465120254,3.4311798487,-0.8748008622  H,2.1437660595,3.4353579015,0.8722323086  C,-3.8610750256,-0.5351996962,-0.002561565  C,-3.6908060558,0.9114291408,-0.0057850869  C,-4.8800451719,1.7245580576,-0.0098824516  H,-4.7565897573,2.8046098288,-0.0122895267  C,-6.1285811274,1.1835860693,-0.010793085  H,-6.9986240253,1.8348137149,-0.0139265428  C,-6.3056114585,-0.2295618513,-0.0076685331  H,-7.3021630417,-0.657086755,-0.0084060659  C,-5.1888132204,-1.0292702982,-0.0037261306  H,-5.3282990808,-2.1070765114,-0.0013481156  C,-1.2623739575,-0.6997924626,0.0024905471  C,-0.041016297,-1.3758230675,0.0063463333  H,-0.0509451119,-2.4647036085,0.0089941664  C,-1.2278174049,0.7420016448,-0.0009682133  C,-2.4366373482,1.4945522351,-0.0049701391  H,-2.3627494858,2.5794837261,-0.0074783788  C,-2.6824113797,-3.0261743341,0.0056286731  H,-2.1617633437,-3.4303706499,0.8811941659  H,-3.6922052664,-3.4440840852,0.0046816805  H,-2.1583129557,-3.4347515745,-0.8658366032  B,-2.6272073962,-1.4212642265,0.0017932908</p>
<p>trans-DBP:CO<sub>2</sub>; E=-1087.50233135H</p>	<p>45  C,0.0931751604,1.416443139,-0.0348436219  C,1.3103997262,0.7311388072,-0.0252476618  C,1.2657272068,-0.7094570018,0.0114913092  C,2.4677160602,-1.4707521637,0.022007508</p>

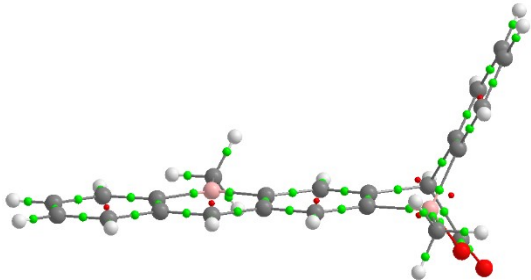


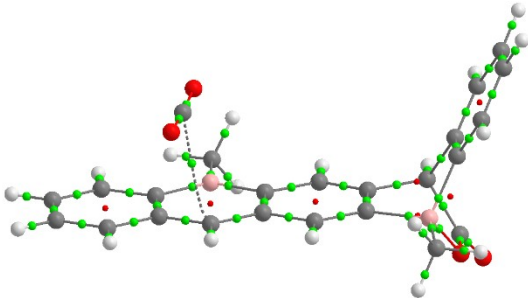
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 C,5.2378927937,1.0320041036,-0.0663248456  
 H,5.3848405423,2.1083160602,-0.0957557717  
 C,6.3484960828,0.2242226664,-0.0549145386  
 C,6.1617191782,-1.1867058014,-0.0158299192  
 C,4.9092494044,-1.7183676768,0.0088937693  
 H,0.1102833704,2.5048127726,-0.0635801408  
 H,2.3860071863,-2.5546172549,0.0511088171  
 H,7.3479843938,0.6443073448,-0.0742982382  
 H,7.0270121556,-1.8440075147,-0.0055836315  
 H,4.778018519,-2.7970081807,0.0387888646  
 B,2.6795387569,1.442855982,-0.0542491342  
 C,2.7460709229,3.0463332514,-0.095650787  
 H,3.7587518377,3.4566905182,-0.110218617  
 H,2.2234336584,3.4341837633,-0.977378418  
 H,2.2303310163,3.4790885261,0.7690055731  
 C,-3.8094160602,-0.4683702295,0.0300092254  
 C,-3.630919333,0.9745626255,-0.0073547094  
 C,-4.813789682,1.7963308698,-0.0100517582  
 H,-4.6835366053,2.8749253098,-0.0291564418  
 C,-6.0655217285,1.2608116572,0.0212804893  
 H,-6.9313612227,1.9172731972,0.0209920962  
 C,-6.2504565745,-0.1489265302,0.0540697077  
 H,-7.2490848057,-0.5704695614,0.0775668603  
 C,-5.1377282064,-0.9556067031,0.0577411413  
 H,-5.2824677535,-2.0320936442,0.0858479154  
 C,-1.2082654554,-0.6502903558,0.0243123156  
 C,0.0065892168,-1.3351660765,0.0360995189  
 H,-0.0109885358,-2.4233490799,0.0658353751  
 C,-1.1633532051,0.7897882006,-0.0136563543  
 C,-2.6443450806,-2.9635505565,0.1009413651  
 H,-2.1307877565,-3.3415591536,0.9920126517  
 H,-3.6560313351,-3.3761054058,0.1069413865  
 H,-2.1167852844,-3.4003453453,-0.7543623694  
 B,-2.5785156233,-1.3617580639,0.0513789677  
 C,-2.3696463876,1.5503924768,-0.0233507958  
 H,-2.2901675841,2.6338973759,-0.0605449061  
 C,-2.8113603819,1.7093881404,2.8374217017  
 O,-2.6054124265,0.5915415058,3.0316810619  
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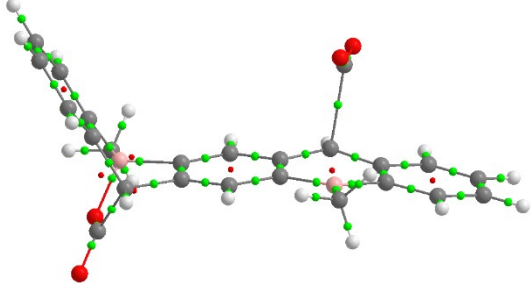
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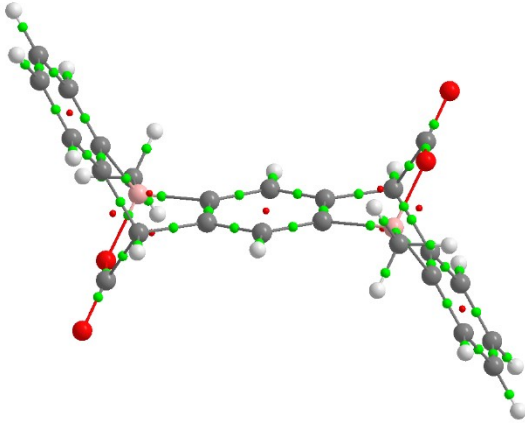
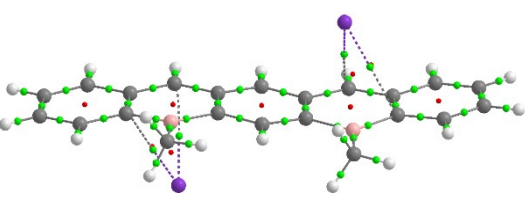


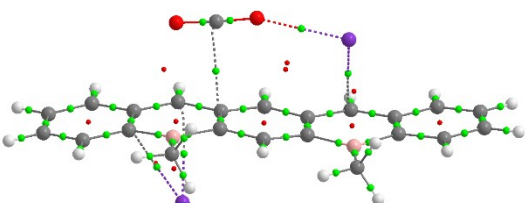
45  
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 C,1.2631345524,-0.4850815465,-0.5359634191  
 C,2.4481856727,-1.1294021697,-0.8930993833  
 C,3.7131056146,-0.525997682,-0.842321196  
 C,-0.0084564793,-1.1615202592,-0.6102760274  
 C,-1.2347212484,-0.4702719656,-0.5027923023  
 C,-1.288095052,0.8870829053,-0.0334334687  
 C,-2.5587989178,1.4848625839,0.0997806443  
 H,-2.6086430113,2.5090581964,0.4572319703  
 C,-3.7346041117,0.8393693445,-0.2120365638  
 C,-3.6692162714,-0.4915769105,-0.6808381948  
 C,-2.4648519157,-1.1235809265,-0.8201935877  
 H,2.6542104715,2.4999877662,0.350224982  
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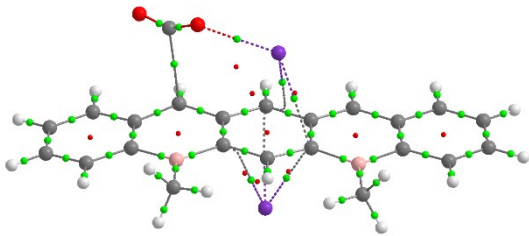
	<p>H,-4.6917014171,1.3364237932,-0.1021897146  H,-4.5843180864,-1.0190269166,-0.9336525622  H,-2.4236437532,-2.1508151752,-1.1678198952  C,0.0830043368,3.0944833477,0.8746059745  H,0.7502905834,3.126187838,1.7414768043  H,0.5117727294,3.786385827,0.1409680879  H,-0.8828499231,3.4989311616,1.1840137789  O,0.0079878616,-1.2032002254,2.1713042955  C,-0.2685712329,-2.054903709,1.4052292558  O,-0.6102161402,-3.1645095059,1.1517767695  B,0.025985674,1.614544587,0.2752584795  C,6.2324998526,0.9228934335,-0.6630404182  C,6.2931409721,-0.4434434612,-1.1544417763  C,7.465997888,1.6574053369,-0.5678030575  C,7.5702428339,-0.9477090068,-1.5044804398  C,8.662334238,1.1125212561,-0.9215593045  H,9.5709401343,1.70186784,-0.8342055192  C,8.7326605582,-0.2235816018,-1.4045826765  H,9.6872028783,-0.6548772729,-1.6848875146  H,7.6290943658,-1.9679206617,-1.8733292613  H,7.4223826508,2.6790202708,-0.199445419  B,5.0068965212,-1.2468803773,-1.2669393875  C,4.9446784069,-2.7604514011,-1.7961384548  H,4.4929196527,-3.4171542974,-1.0445522941  H,4.3029141064,-2.8365790989,-2.681156724  H,5.9150472224,-3.1874759251,-2.0606659299  C,5.0315781717,1.5096158758,-0.2969406925  H,5.0365559431,2.5351010209,0.0638374243</p>
<p>trans-DBP-CO<sub>2</sub>; E=-1087.55068567H</p> 	<p>45  C,0.0799960435,-0.6331482254,-1.28641995  C,1.3054765777,-0.1252016338,-0.9594341785  C,1.3502879566,0.9993633322,-0.0840189009  C,3.5243061633,0.2962237246,0.8378418682  C,3.5663066685,-0.8409595349,0.012522572  C,4.2225695391,-1.9657203757,0.4932269651  H,4.269403937,-2.8594292044,-0.1232317719  C,4.825372845,-1.9693106686,1.7530171446  C,4.7780910243,-0.8335199654,2.5482762962  C,4.1248458223,0.3090395176,2.0855432652  H,0.0113729974,-1.4903903432,-1.9548076089  H,5.3323491557,-2.8589141757,2.1130987625  H,5.2443226262,-0.8330870428,3.5276327367  H,4.0792521401,1.200801263,2.7028228167  B,2.7998980976,-0.5786573793,-1.4034367355  C,2.9443426253,-1.7182710302,-2.5297415199  H,3.9929463459,-1.9202333057,-2.7761209955  H,2.4968276005,-2.6603903608,-2.1935394135  H,2.4353426925,-1.4305614022,-3.4549416788  C,-3.6743442077,0.9891797224,0.188053961  C,-3.6045032532,-0.152647987,-0.6987537659  C,-4.8347119892,-0.7700378428,-1.1021205704  H,-4.7803150825,-1.6273012991,-1.7679651451  C,-6.0476888255,-0.3140013275,-0.6764530003  H,-6.9573465561,-0.8092464978,-1.0042607025  C,-6.1280024767,0.8041041225,0.1927133017  H,-7.092717052,1.1663360566,0.5308055199  C,-4.9624646929,1.4132700094,0.593265424  H,-5.0308817404,2.2691067987,1.2589833265  C,-1.0845638653,1.055576106,0.0860011347</p>

	<p>C,0.2071623894,1.5634475793,0.4071252757  H,0.2778804639,2.4245934081,1.0689929972  C,-1.1432719406,-0.0784830259,-0.7861809251  C,-2.3280333236,2.933851151,1.6115989418  H,-1.8159338797,3.7768761156,1.1345753392  H,-3.3089684064,3.2924448207,1.9337585181  H,-1.7532034077,2.7081579072,2.5168772388  B,-2.3751873989,1.661003694,0.6297526893  C,2.765894729,1.4640940583,0.2346605288  H,2.7894144937,2.3544627908,0.8605032721  C,3.4519742706,1.7603245404,-1.1076699814  O,3.9418396237,2.843635695,-1.3696275206  O,3.4623837056,0.7381683795,-1.9180151009  C,-2.3827335618,-0.6449397868,-1.151971031  H,-2.3808558742,-1.504691378,-1.8171463992</p>
<p>trans-DBP-CO<sub>2</sub>:CO<sub>2</sub>; E=-1276.15852733H</p> 	<p>48  C,0.0728954494,-0.6347184805,-1.2893260057  C,1.2987343619,-0.1293748859,-0.9570272154  C,1.3430979168,0.9934755972,-0.0805783089  C,3.5166647607,0.2886623978,0.8422886417  C,3.5586052566,-0.8471766345,0.0155656746  C,4.2151065255,-1.9725517568,0.4943939458  H,4.2616976829,-2.8654221345,-0.1232258838  C,4.8184531585,-1.9774901626,1.7538486118  C,4.7714705348,-0.8426609348,2.5505077038  C,4.1178391766,0.3003281952,2.0896868601  H,0.0043086303,-1.4900222953,-1.9600040497  H,5.3255206194,-2.867540271,2.1125082925  H,5.2378920871,-0.8435670461,3.5297132868  H,4.0723965464,1.1912450429,2.7081289271  B,2.793724845,-0.5831130511,-1.4002678052  C,2.9380137702,-1.7196567676,-2.529146466  H,3.9868142949,-1.9235048822,-2.7728845257  H,2.4870126795,-2.661921975,-2.1982905323  H,2.4331500577,-1.4271258009,-3.455102468  C,-3.6844824416,0.9960035491,0.1729683644  C,-3.6159459024,-0.1435183142,-0.7142356687  C,-4.8448929597,-0.7678042627,-1.1099774889  H,-4.7902356867,-1.6304384973,-1.7680894878  C,-6.0568282514,-0.3156029145,-0.674327847  H,-6.9661942313,-0.8166629548,-0.993352125  C,-6.1360079703,0.8033991374,0.1914099233  H,-7.0998034719,1.1618415,0.5355834346  C,-4.9699941362,1.4176015507,0.5846990218  H,-5.0367265489,2.2725067356,1.2513306058  C,-1.0912471929,1.0550971928,0.0802699493  C,0.199378135,1.5596520796,0.4075782872  H,0.2694036085,2.4193372176,1.0710679974  C,-1.1492033645,-0.0762293527,-0.7928554784  C,-2.3356088531,2.9274391484,1.6096802666  H,-1.8015819046,3.7650667416,1.1478593896  H,-3.3160832313,3.2989323484,1.9175234606  H,-1.780422567,2.6844493002,2.5225355664  B,-2.3831258889,1.6620298928,0.6213121487  C,2.7582779707,1.4574825117,0.2406940582  H,2.7808638902,2.3468645947,0.8678876009  C,3.4447626275,1.7559400718,-1.1010328352  O,3.9343390297,2.839628324,-1.3610206042  O,3.4551646209,0.7348819265,-1.9127156945</p>

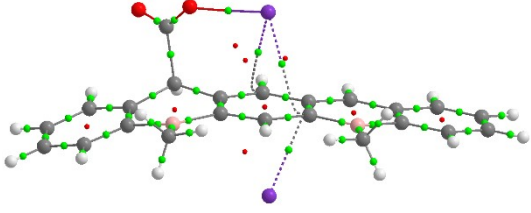
	<p>C,-2.3909815329,-0.6414990524,-1.1618526903  H,-2.3902167796,-1.4946573749,-1.8348593734  C,-2.8334878982,-2.4971697382,1.0617085456  O,-2.5580441776,-1.7381546814,1.884553867  O,-3.1235302456,-3.3432248341,0.3222241226</p>
<p>trans-DBP-CO<sub>2</sub>/CO<sub>2</sub>; E=-1276.15080997H</p> 	<p>48  C,0.1009596009,0.2911418448,-1.3976853894  C,1.3001203311,0.5226298171,-0.7704923233  C,1.3003048384,0.6383252091,0.6426878552  C,3.5950300098,-0.2526273322,0.7987810888  C,3.6854447147,-0.4009951864,-0.5951135381  C,4.4861335525,-1.4221272859,-1.0874900387  H,4.5720161071,-1.5614591188,-2.1615063614  C,5.1837142076,-2.2719806272,-0.2270856441  C,5.0867363394,-2.1022839557,1.1464080679  C,4.2881995333,-1.0824186342,1.6636506064  H,0.0674320646,0.1945464592,-2.4810105161  H,5.8025031092,-3.0673635519,-0.6295993522  H,5.6258606993,-2.7623013286,1.8170992317  H,4.2029517252,-0.9452462285,2.7369789122  B,2.7960796943,0.7210284284,-1.3743209238  C,2.9621920689,0.807282167,-2.9704855904  H,4.0047935578,0.972743619,-3.2639535077  H,2.6268962066,-0.1182788969,-3.4512257917  H,2.3665407007,1.6238552433,-3.390201339  C,-3.7259514478,0.2459280521,0.6452094612  C,-3.617865939,0.1293855107,-0.7709108304  C,-4.8055193094,0.1493022215,-1.5491696875  H,-4.7178652883,0.0487714363,-2.6260704911  C,-6.0398481605,0.2773771405,-0.9646729341  H,-6.9301162347,0.2931980288,-1.5856980436  C,-6.1599973895,0.3861686763,0.4332221949  H,-7.1370800424,0.4846625516,0.8926636396  C,-5.0146719859,0.3635753072,1.2004650657  H,-5.1037841475,0.446599863,2.2802629453  C,-1.1117481754,0.3210238609,0.7340021421  C,0.1408345631,0.5398565895,1.3642334202  H,0.1771883209,0.6428573643,2.4455674441  C,-1.1214362721,0.1914483743,-0.6804946868  C,-2.5387053947,0.3018863628,3.0895099111  H,-2.9540109262,1.258251768,3.4284922829  H,-3.2186846171,-0.4737459451,3.4560694283  H,-1.5812511914,0.1667825009,3.5945593319  B,-2.4391401964,0.2655873627,1.4947674663  C,2.6818865162,0.8775793872,1.2368005015  H,2.662011228,1.0149428697,2.3163650025  C,3.2356402468,2.1450568001,0.5663752051  O,3.5963824312,3.1180131517,1.2018012758  O,3.2838391608,2.0590443974,-0.733909348  C,-2.3470287314,-0.0594184395,-1.3902257131  H,-2.3093726859,0.0386875573,-2.4689436958  C,-2.4941253111,-2.1750789361,-1.4303095969  O,-2.3434641477,-2.5657128633,-0.3227394377  O,-2.7038959539,-2.4247265723,-2.5792001602</p>
<p>trans-DBP-(CO<sub>2</sub>)<sub>2</sub>; E=-1276.19616372H</p>	<p>48  C,0.0273551582,1.3613059174,-0.2474478042  C,1.1076403062,0.781928889,0.414370363  C,1.0618006807,-0.5959222795,0.6489069274  C,3.5209294391,-0.7863886504,0.5261909627</p>

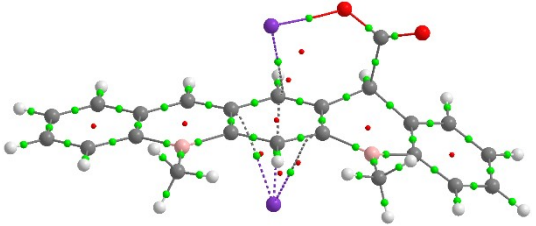
	<p>C,3.6624112365,0.5899741833,0.2835233294  C,4.7441743091,1.0053364505,-0.4796600932  H,4.8786711956,2.0641798424,-0.6832287872  C,5.6641643247,0.0863554248,-0.9897999393  C,5.5098029792,-1.2674676789,-0.730957731  C,4.4314406635,-1.7073186468,0.0376204879  H,0.0233421686,2.4307817026,-0.4483706696  H,6.5015713251,0.4284758704,-1.5893373126  H,6.2214437155,-1.9836266296,-1.1269717288  H,4.3011139474,-2.7651634087,0.2427708136  B,2.4709054107,1.4427507367,1.0011344548  C,2.6058594308,3.0451906259,0.9799232168  H,3.5476148023,3.3812547266,1.4279294291  H,2.5739713761,3.4291840078,-0.0459295012  H,1.7890803735,3.5227814201,1.5302161281  C,-3.653452677,-0.6073851152,-0.2775194289  C,-3.5119485811,0.7689869593,-0.520139267  C,-4.4223832158,1.689924296,-0.0314446329  H,-4.2920380031,2.7477755256,-0.2365432087  C,-5.500703351,1.2500651964,0.7371893679  H,-6.2122844743,1.9662301422,1.1333001668  C,-5.6550948298,-0.1037647296,0.9959752407  H,-6.4924668418,-0.4458789407,1.5955649681  C,-4.7351717657,-1.0227520861,0.4857278612  H,-4.8696781262,-2.0816016755,0.6892512936  C,-1.0986791083,-0.7993605151,-0.4083854939  C,-0.0184048226,-1.3787409947,0.2534360944  H,-0.0144107325,-2.4482083044,0.4544015136  C,-1.0528251633,0.5784786631,-0.6429598032  C,-2.5965422673,-3.0626521381,-0.9738721955  H,-2.564404523,-3.4465861383,0.051996681  H,-3.5381409874,-3.399211212,-1.4218214691  H,-1.7795325066,-3.5398628384,-1.5241628023  B,-2.4620009713,-1.4601827855,-0.9951687143  C,2.2988754152,-1.1387904195,1.3555337648  H,2.2294816255,-2.2014780265,1.5799047439  C,2.448868997,-0.3454737535,2.6646374446  O,2.4963411744,-0.8851622641,3.7540789675  O,2.534672408,0.9418432609,2.4784032081  C,-2.2899253117,1.1213527909,-1.3495531176  H,-2.2205411838,2.1840369588,-1.5739540694  C,-2.4401969335,0.3280412507,-2.6586109635  O,-2.5257346628,-0.9593103018,-2.4723753131  O,-2.488212873,0.8677379612,-3.7480253526</p>
<b><i>cis</i>-Diborapentacene<sup>(2-)</sup>·2K<sup>+</sup></b>	
<p><i>cis</i>-DBP-K<sub>2</sub>; E=-2098.82118906H</p> 	<p>44  C,0.0897055502,1.301162814,-0.005173367  C,1.278888168,0.5592962706,-0.0883098275  C,1.1991311123,-0.8933634282,-0.0915616186  C,3.7916409452,-0.9659491272,-0.0416532916  C,3.7556381954,0.4774814931,-0.0649248  C,5.0006356796,1.1838344284,-0.0007636078  H,4.979208581,2.2680195338,-0.0327116475  C,6.1915176812,0.5264643502,0.0924940265  C,6.2379193539,-0.888021926,0.1251964445  C,5.0643054831,-1.5897556405,0.0526683433  H,0.1543936103,2.386331,-0.006552238  H,7.1143846882,1.0932651303,0.136336469</p>

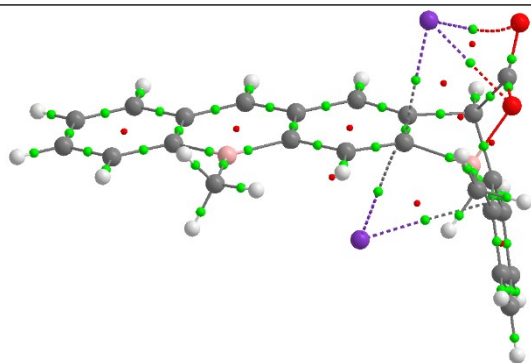
	<p>H,7.1890622578,-1.39923557,0.1933043639  H,5.1030672401,-2.6732792819,0.0642401379  C,-3.8591141857,-0.4859189583,0.0378763404  C,-3.6490622052,0.9391586388,0.0556302866  C,-4.7991786959,1.7899163303,-0.009589829  H,-4.648419522,2.8640182293,0.0149451111  C,-6.0612790189,1.2785129749,-0.0928611654  H,-6.9098241807,1.9514720802,-0.1369793811  C,-6.2777208804,-0.1199907413,-0.1141647299  H,-7.2840432192,-0.5132299156,-0.1726817821  C,-5.195310383,-0.9568886262,-0.0443984773  H,-5.357903661,-2.0300819656,-0.0451417628  C,-1.278829607,-0.7475869351,0.0851501417  C,-0.0762516329,-1.4607859833,-0.0034502053  H,-0.1355893229,-2.5452729442,-0.0058236056  C,-1.1817115425,0.7072125514,0.0789466181  C,-2.3583120222,1.4930937702,0.0825081154  H,-2.2580140843,2.5737810716,0.1023080207  C,-2.8598935706,-3.0067411191,0.2104869823  H,-3.4864323897,-3.2680733285,1.0688966991  H,-3.3944006921,-3.3885090894,-0.6661836694  H,-1.9386416591,-3.5827936692,0.2988530475  B,-2.6565113827,-1.4285065021,0.138217524  K,-2.3400319563,0.1825873368,-2.4679946685  K,2.360181268,-0.1045058466,2.4596318878  C,2.3958836302,-3.3361542761,-0.2012445044  H,1.9216722799,-3.7532230303,0.6942169763  H,1.7711228991,-3.6606276184,-1.0386743921  H,3.3603630958,-3.8319899115,-0.3112442581  B,2.4791153485,-1.7461952574,-0.1414806777  H,2.5848121289,2.2745665725,-0.1173470705  C,2.5462988974,1.189972146,-0.094433119</p>
<p>cis-DBP-K<sub>2</sub>:CO<sub>2</sub>; E=-2287.43309602H</p> 	<p>47  C,-6.162898,-0.148532,0.262982  C,-5.032425,-0.212131,1.033289  C,-3.721465,-0.124285,0.494696  C,-3.596004,0.045254,-0.933152  C,-4.796164,0.122186,-1.711047  C,-6.028426,0.026471,-1.134852  C,-2.344576,0.0826,-1.570256  C,-1.118869,-0.069543,-0.875634  C,-1.128729,-0.19574,0.575354  C,0.10644,-0.399733,1.203285  H,0.100508,-0.489524,2.285636  C,1.340606,-0.502731,0.552724  C,1.33155,-0.38,-0.900266  C,0.104256,-0.173321,-1.555154  H,-7.145735,-0.216032,0.710291  H,-5.138164,-0.330986,2.105753  H,-4.706786,0.264166,-2.782833  H,-6.915816,0.091108,-1.753842  H,-2.316027,0.205714,-2.648501  H,0.105366,-0.079471,-2.638186  B,-2.455966,-0.161883,1.354275  C,-2.464949,-0.233758,2.945385  H,-2.002493,-1.154507,3.316992  H,-1.869541,0.581037,3.369666  H,-3.456481,-0.16897,3.393117  C,-1.078023,2.857377,0.208853</p>

	<p>O,-2.215576,2.914078,0.342514  O,0.078145,2.869379,0.083068  C,3.803191,-0.521421,-0.994623  C,3.929046,-0.630065,0.435578  C,5.00255,-0.480011,-1.774788  C,5.236773,-0.68733,0.982513  C,6.235285,-0.534285,-1.191857  H,7.123099,-0.504124,-1.812928  C,6.369375,-0.63718,0.212786  H,7.352166,-0.68631,0.662761  H,5.335146,-0.780445,2.059438  H,4.914283,-0.40939,-2.853763  K,2.652704,2.053895,-0.115223  C,2.772397,-0.905847,2.878424  H,3.337207,-0.095922,3.352806  H,1.815055,-0.97249,3.395529  H,3.327152,-1.820584,3.108758  C,2.548345,-0.406818,-1.617925  H,2.51217,-0.336071,-2.700474  B,2.668605,-0.705129,1.301827  K,-2.346313,-2.600039,-0.538107</p>
<p>cis-DBP-K<sub>2</sub>/CO<sub>2</sub> (TS1); E=-2287.42298318H</p> 	<p>47  C,-6.1319267086,0.6273412541,-0.5743111933  C,-5.0463437388,0.082152798,-1.2139452618  C,-3.7273518551,0.2167264884,-0.7238682363  C,-3.5349950412,0.9524005154,0.4852918175  C,-4.6719826633,1.508708191,1.1314821739  C,-5.9304014427,1.3505440941,0.6172565734  C,-2.2453487385,1.1364110635,1.0483091027  C,-1.0863513265,0.6216265645,0.4753979261  C,-1.1600004232,-0.1485581649,-0.7707328303  C,0.0574308593,-0.62304,-1.2938182122  H,0.0085532116,-1.1863987179,-2.2201893922  C,1.319808081,-0.4484337139,-0.7182939927  C,1.3841353609,0.3002901504,0.5362182629  C,0.1981753638,0.8150689092,1.0705141811  H,-7.1302571708,0.5071944366,-0.9744404239  H,-5.2004671234,-0.4747522933,-2.13226493  H,-4.5273088631,2.0679889233,2.0493685615  H,-6.7794845297,1.7856935532,1.1310030126  H,-2.1630305203,1.7043989376,1.969511174  H,0.2505094398,1.3840080608,1.9957966284  B,-2.5200250331,-0.3926290915,-1.4429277191  C,-2.6987074165,-1.2154268479,-2.7934279522  H,-1.7785146254,-1.6085934843,-3.2273391564  H,-3.3710500645,-2.0659000765,-2.6425587368  H,-3.1778424551,-0.5998523977,-3.5612403452  K,0.2085615728,2.3647239399,-1.4609763872  C,3.8265137809,-0.1826577579,0.7501602419  C,3.8720822705,-0.9304169118,-0.4607398622  C,4.9987781473,-0.0983600059,1.5389475267  H,4.9703461986,0.4776021739,2.4563338442  C,5.0891010322,-1.5431181657,-0.8214840346  H,5.1293540902,-2.109534235,-1.7459801911  C,6.1611239714,-0.7170798653,1.1511314196  H,7.0437808884,-0.6342969837,1.7743516345  C,6.2201186496,-1.4514192563,-0.0434088075  H,7.1414427517,-1.9337102336,-0.3425550085  K,-0.2341207966,-2.0382976862,1.2874012829</p>



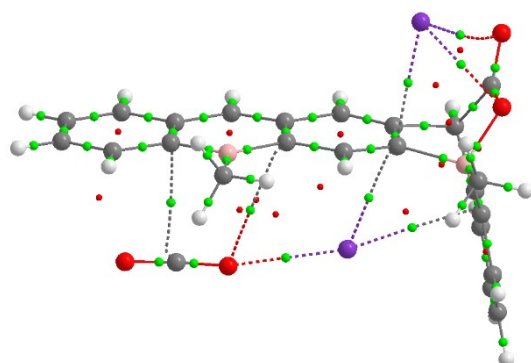
	<p>B,2.6038171682,-1.0647395103,-1.3153832403  C,2.6326326523,-1.8369425229,-2.7017858167  H,2.8940559774,-2.8894172787,-2.5501433823  H,1.7034213038,-1.8149759935,-3.2717436393  H,3.4186470375,-1.4324359223,-3.3460890865  C,2.6403776661,0.5081570978,1.1662459116  H,2.6293526344,0.9126675908,2.1732107643  C,3.2804210291,2.5809476682,0.4086242861  O,4.1403066567,2.8434670913,1.1523119219  O,2.5451167406,2.7967976148,-0.4995304091</p>
<p>cis-DBP-K<sub>2</sub>-CO<sub>2</sub> (inte1); E=-2287.44092597H</p> 	<p>47  C,6.1256473206,0.5142593541,0.3524353358  C,5.0441135811,0.1282175792,1.1047533639  C,3.7130166787,0.2870334882,0.6557583553  C,3.5118891235,0.8703270227,-0.6291253474  C,4.6411912975,1.2651448517,-1.3906328142  C,5.9128402479,1.0916138295,-0.9130136481  C,2.203652635,1.0601840441,-1.1587105899  C,1.060365682,0.6908981944,-0.4750953159  C,1.1382486221,0.0687602095,0.8439974852  C,-0.0765620415,-0.3721165551,1.4125870676  H,-0.0225182152,-0.8595079825,2.3812331283  C,-1.3293655617,-0.2609609907,0.8138282943  C,-1.3953827726,0.4200042594,-0.4632167077  C,-0.2478358808,0.8643656159,-1.0607843718  H,7.1334268577,0.3815851887,0.7241683031  H,5.2110138054,-0.3132122512,2.0813585837  H,4.4829417816,1.7129732369,-2.3654323839  H,6.7606599624,1.4022377647,-1.511488361  H,2.1049696846,1.5252667875,-2.1341655179  H,-0.3147900104,1.3859460693,-2.0124359165  B,2.506742702,-0.1458114824,1.5009784443  C,2.7037596494,-0.7890889757,2.9415631878  H,1.7828961127,-1.0480561028,3.4654353901  H,3.3098011102,-1.6990014208,2.8864566714  H,3.2607679667,-0.1083194504,3.5927409853  K,-0.4375074358,2.6712939169,1.4145978656  C,-3.8503123889,-0.1810119696,-0.7196091138  C,-3.8459155431,-0.9268524576,0.4733976658  C,-4.9618392022,-0.2260346121,-1.5629374129  H,-4.9704633885,0.3924209835,-2.4514742696  C,-4.9708996223,-1.7121989613,0.7707335989  H,-4.9840030055,-2.2859342665,1.6909239316  C,-6.0517959655,-1.0172560865,-1.2480359204  H,-6.906396134,-1.041802909,-1.9129261156  C,-6.060442904,-1.7713419194,-0.0767577812  H,-6.9165630333,-2.3861917658,0.1697653008  K,0.3671791376,-2.0140937234,-1.0299578306  B,-2.6120391856,-0.8770250028,1.41423832  C,-2.6738916625,-1.5118119318,2.8582607917  H,-2.8205360126,-2.5954282095,2.7908328244  H,-1.7965076345,-1.3409092183,3.4816676372  H,-3.5460987729,-1.1341783051,3.3989343656  C,-2.721508667,0.7434923452,-1.0740363271  H,-2.6286639575,0.8000988947,-2.1593013951  C,-3.1797547842,2.2323097839,-0.6599064652  O,-4.0154613755,2.7298988954,-1.3935872625  O,-2.6193088012,2.6970502347,0.3662069706</p>

<p>cis-DBP-K<sub>2</sub>/CO<sub>2</sub> (TS2); E=-2287.43784998H</p> 	<p>47  C,5.74304055,-1.4076884646,0.1753371354  C,4.6872751068,-1.182765866,1.0429709113  C,3.5722666319,-0.4267669511,0.6616113896  C,3.5482596421,0.1235566931,-0.6342073894  C,4.6194880751,-0.0879454595,-1.495052909  C,5.7054284407,-0.8532152512,-1.0988425896  C,2.4144915034,1.0093651705,-1.056458923  C,1.0922747469,0.5986598264,-0.4948800053  C,1.0484245302,0.214523906,0.9040937183  C,-0.2100661904,0.0719722275,1.4817152385  H,-0.2550017678,-0.1824555625,2.5365785251  C,-1.4358678415,0.1774562637,0.7873058256  C,-1.3635397264,0.4667809854,-0.642806516  C,-0.0584951633,0.7038746642,-1.2195838722  H,6.5954802254,-1.9968148092,0.4884079582  H,4.7273574202,-1.5978258382,2.0442612003  H,4.6091586113,0.3666490628,-2.4788703826  H,6.5313702867,-1.0093432537,-1.781783811  H,2.3576120952,1.0673770584,-2.1456054604  H,-0.0056632139,1.0144871882,-2.2590163007  B,2.3631919515,-0.1819914287,1.6133192896  C,2.4747270372,-0.4540085072,3.161312386  H,2.7305731524,-1.5003865737,3.3586296736  H,1.5814624682,-0.2181753545,3.7396084048  H,3.3033925762,0.1299263171,3.5726611011  C,2.6666686485,2.5303276077,-0.577231544  O,3.7610561925,2.7877548126,-0.1072412658  O,1.664776329,3.2752989717,-0.7468938866  C,-3.8051241618,0.2568695034,-0.8974373237  C,-4.0029130089,-0.0239854633,0.4849358022  C,-4.9281080149,0.2955184516,-1.7608204685  C,-5.3251027299,-0.2554278001,0.9257587581  C,-6.1929922278,0.0642483291,-1.2876175862  H,-7.0372676005,0.0997868709,-1.9653908089  C,-6.4022631369,-0.2168304693,0.0742208039  H,-7.4041289687,-0.3970839685,0.4419388999  H,-5.4902661927,-0.4693596695,1.9761666385  H,-4.7722438563,0.5140626463,-2.8114531261  K,-0.3953629112,3.1110349549,0.5471162649  C,-2.9972986342,-0.3708121092,2.988656426  H,-3.6793979608,0.3576205656,3.4379318042  H,-2.0840841984,-0.3611568608,3.584601464  H,-3.4716163308,-1.3455800082,3.1407974892  C,-2.5021592416,0.4977297605,-1.4234828292  H,-2.4077397151,0.724874092,-2.480468787  B,-2.799800165,-0.0687243734,1.4407823202  K,-0.1536832625,-2.1434888874,-0.5071926434</p>
<p>cis-DBP-K<sub>2</sub>-CO<sub>2</sub>; E=-2287.47007621H</p>	<p>47  C,3.4907847932,-3.3806163763,0.6129345654  C,3.4218390394,-2.152001087,1.2739647365  C,3.2325156387,-0.9684367958,0.5675509141  C,3.1277551803,-1.0485277398,-0.8318696393  C,3.2119554327,-2.2596431178,-1.5023716411  C,3.3893004645,-3.4353048162,-0.7716140143  C,2.7239589018,0.2480957342,-1.5031972815  C,1.3549440621,0.5777032375,-0.8934802549  C,1.4032072602,0.755544269,0.5335868435  C,0.1964323112,0.9184715889,1.1786708656</p>

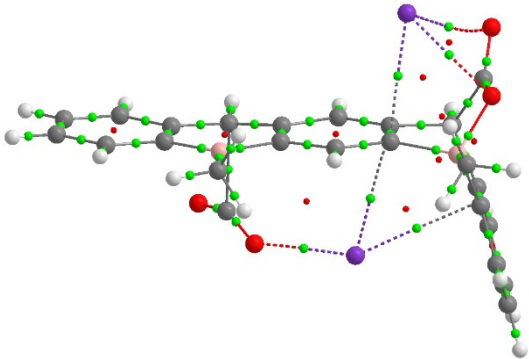


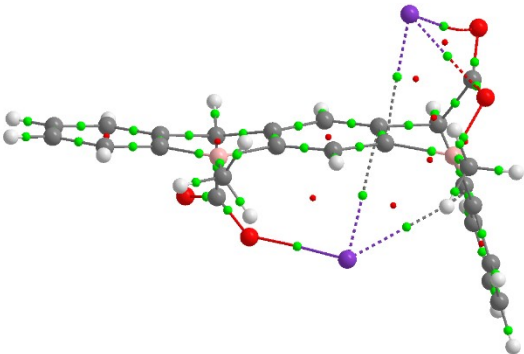
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 C,-1.0804211638,0.6535840717,-0.907211138  
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 H,3.5106957481,-2.1216538189,2.355183896  
 H,3.1284937778,-2.2963397476,-2.5830642496  
 H,3.4572487935,-4.3860202384,-1.2849343875  
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 C,3.1728185947,0.8350763515,2.665258409  
 H,2.569043847,0.1935501338,3.3146196276  
 H,2.9198811743,1.8667120101,2.9353299736  
 H,4.2193630084,0.6799048678,2.9394690217  
 C,3.568667366,1.4292177738,-1.0517079564  
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 C,-3.5303796868,0.5131090848,-0.983789311  
 C,-3.6517571916,0.7059089013,0.425300345  
 C,-4.7081723565,0.3314109238,-1.7589458892  
 C,-4.9558724424,0.7036089422,0.9759727889  
 C,-5.9464199181,0.3368595385,-1.1793669885  
 H,-6.8301291403,0.1978487639,-1.7907703783  
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 H,-7.0640502596,0.5297151459,0.6641869744  
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 K,2.0592125428,3.5341288253,0.0099545623  
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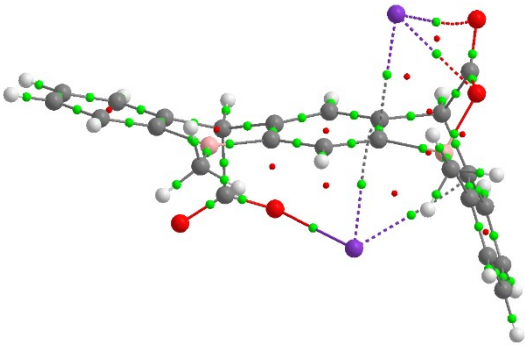
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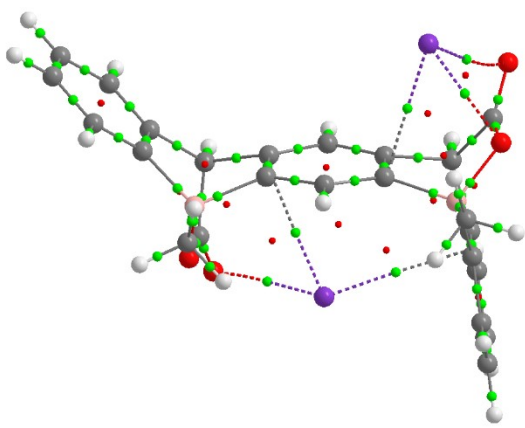


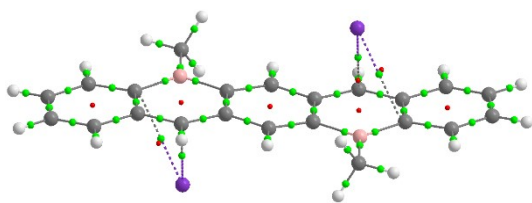
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 H,2.4774655092,1.9152237182,-2.5047134936  
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	<p>C,2.851509628,1.5502483028,2.7827521678  H,2.5836242784,0.5970394777,3.2491542416  H,2.2124927804,2.3090256,3.2484307768  H,3.8804980907,1.7753493666,3.0743666024  C,2.8318121588,3.0361938183,-0.6991591286  O,3.0456481712,2.8959321434,0.5818309566  O,2.6736646486,4.1302205742,-1.2154010116  C,-3.3872300435,-0.4000295433,-1.1843156235  C,-3.5141853272,-0.6034351226,0.2258074579  C,-4.4685884366,-0.7700580555,-2.0331611474  C,-4.7245089768,-1.1689358076,0.6989240804  C,-5.6153542533,-1.311889125,-1.5253091704  H,-6.4247379396,-1.585134616,-2.1917461723  C,-5.7533113296,-1.518756155,-0.1365213385  H,-6.6648019587,-1.9492708663,0.2579089935  H,-4.8355232245,-1.3264424488,1.7666728507  H,-4.368288048,-0.6104630625,-3.1014217054  K,0.6067987448,4.0615455646,0.6541213592  C,-2.5087590274,-0.4027207418,2.7427709892  H,-3.3774045631,0.1375983674,3.1321878499  H,-1.6453807764,-0.0783841972,3.3254321303  H,-2.6836022795,-1.4550160092,2.9899967927  C,-2.2115510199,0.1554163221,-1.7389894124  H,-2.1591868448,0.2944544463,-2.8139104883  B,-2.3759984357,-0.1946820822,1.1672785693  K,1.1762744467,-1.5337766627,-0.3302151432  C,-2.2219338726,-3.2771734017,-0.7734110718  O,-1.1260180276,-2.9124892109,-0.6387340153  O,-3.2753270414,-3.707842245,-0.9155088453</p>
<p>cis-DBP-K<sub>2</sub>-CO<sub>2</sub>/CO<sub>2</sub> (TS1); E=-2476.07172676H</p> 	<p>50  C,4.9439170422,-1.4806508828,0.1141649993  C,4.3186526882,-0.5559656101,0.9534843173  C,3.5392633045,0.4695856128,0.4298147658  C,3.4157411614,0.5556772559,-0.966288795  C,4.0447655447,-0.3448738339,-1.8121576596  C,4.8090669658,-1.3753483392,-1.2641653217  C,2.4190691166,1.5921810435,-1.443874791  C,1.0772198739,1.1827128177,-0.8238597686  C,1.1083199105,1.1331855642,0.6007047024  C,-0.0326192268,0.6781209937,1.2314293391  H,-0.0394260235,0.6216098556,2.318513455  C,-1.1861747024,0.2337524061,0.5350603257  C,-1.1811106345,0.2984097132,-0.8897713167  C,-0.0226336006,0.8071462066,-1.5482622224  H,5.5457322204,-2.2765678898,0.5354382672  H,4.4380223543,-0.6433965015,2.0285617126  H,3.9347654191,-0.2596240472,-2.8874915014  H,5.3015731931,-2.0868248437,-1.9144636921  H,2.3680311731,1.6938133267,-2.5248258545  H,-0.0078345146,0.8453435612,-2.6340765742  B,2.5786036616,1.5274146597,1.193752316  C,2.7293799316,1.6983247711,2.7742261984  H,2.5183888139,0.7618852842,3.3000019734  H,2.0381591539,2.4424303313,3.1861615704  H,3.738519696,2.0074834896,3.0575150764  C,2.6498319637,2.9506153103,-0.7974097323  O,2.8609128729,2.9067556969,0.491782739  O,2.4357540571,3.9982050339,-1.3836558127  C,-3.482542529,-0.6392748822,-1.0380349804</p>

	<p>C,-3.6072928786,-0.7336213719,0.375554297  C,-4.5847913107,-0.9843063493,-1.8537918031  C,-4.8411978758,-1.1817361753,0.8977928911  C,-5.765714821,-1.4082424313,-1.3009039956  H,-6.5978388782,-1.6666964218,-1.9447382108  C,-5.903983146,-1.5121617318,0.0928015237  H,-6.838625227,-1.8491280607,0.5220933904  H,-4.9543347044,-1.2619505032,1.9722623587  H,-4.4778975459,-0.9195220352,-2.9299577366  K,0.4012563898,3.9910775395,0.4957503203  C,-2.4367532924,-0.4255303271,2.8510989642  H,-3.3357363977,-0.8740360462,3.2714614049  H,-2.3284221535,0.5652386052,3.3052039045  H,-1.5856014815,-1.0103673026,3.2143905148  C,-2.2489336953,-0.2340572417,-1.6562501753  H,-2.2874880912,0.0340827259,-2.7057878428  B,-2.4284647205,-0.3244000744,1.2667372903  K,1.3708091524,-1.7224093472,-0.1159476266  C,-1.5426028271,-2.2209751458,-2.1438943333  O,-0.749045037,-2.5231606876,-1.3014325279  O,-2.1186913451,-2.4802247211,-3.1347153432</p>
<p>cis-DBP-K<sub>2</sub>-CO<sub>2</sub>-CO<sub>2</sub> (inte1); E=-2476.08282227H</p> 	<p>50  C,4.0639228338,-2.7662400906,1.2715361492  C,3.792150201,-1.4452072132,1.6337505186  C,3.3137236319,-0.5355182195,0.6985137567  C,3.1283627638,-0.9811529176,-0.6194546056  C,3.4115223461,-2.2840085055,-0.9982231872  C,3.8766481235,-3.184309585,-0.039482937  C,2.4546598371,0.0259023185,-1.5316799649  C,1.1059634361,0.3379250651,-0.8716283602  C,1.2248464956,0.8648782965,0.4341594599  C,0.0495473025,1.085709402,1.1329649912  H,0.1076985071,1.4932473856,2.1398043889  C,-1.2210102975,0.745123227,0.6148425996  C,-1.2909379682,0.1808581471,-0.667590984  C,-0.1162771569,0.0214303371,-1.4241753929  H,4.43172623,-3.4670049528,2.0108506665  H,3.9508492533,-1.1284559623,2.6593008166  H,3.2588883701,-2.6066569868,-2.0219181077  H,4.0949734212,-4.2064920942,-0.3205562424  H,2.3515474029,-0.3066073562,-2.5611406063  H,-0.1775149896,-0.428349918,-2.4109430986  B,2.7862999762,0.9815546752,0.9089674842  C,3.0966597486,1.7236858296,2.2881871687  H,2.6445800511,1.197632246,3.1345052884  H,2.7027305408,2.7465599935,2.3193557578  H,4.1696453499,1.7886992399,2.4841236608  C,3.1435614048,1.3805711739,-1.4798669992  O,3.4345573129,1.7917261219,-0.2723021086  O,3.2228065695,2.1182401498,-2.4473641267  C,-3.8222400283,-0.0260640073,-0.5459678633  C,-3.8562967326,0.599892914,0.7147818142  C,-5.0166845554,-0.3387736637,-1.2007398684  C,-5.1117515811,0.9063709196,1.2693668651  C,-6.2333773268,-0.0177799162,-0.6314248121  H,-7.1503157484,-0.2641542005,-1.1526280956  C,-6.2878039828,0.6145288407,0.6103329691  H,-7.2431827333,0.8643879493,1.0534945974  H,-5.1582369283,1.3893837238,2.2377129057</p>

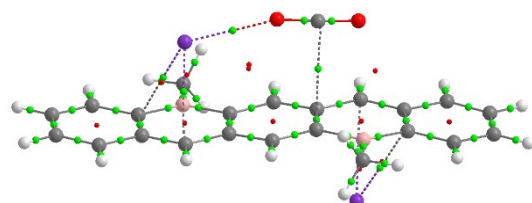
	<p>H,-4.9710280249,-0.8593198723,-2.1487793219  K,1.5906841141,3.6020335946,-0.8155212882  C,-2.4572399037,1.4927717517,2.9113638213  H,-3.4112410224,1.5475384275,3.4321175999  H,-2.0175307808,2.4961222159,2.9205694425  H,-1.7867546354,0.8750280552,3.5169016776  C,-2.5373403618,-0.4307486751,-1.1971497157  H,-2.6091871029,-0.2753428816,-2.2742130155  B,-2.5353113336,0.9398898932,1.4360474797  K,0.5737646782,-2.1770583761,0.8234694174  C,-2.4201190731,-2.0469161562,-1.0641290642  O,-1.6440049217,-2.4480601774,-0.1618520078  O,-3.1011668427,-2.6715555463,-1.8573640029</p>
<p>cis-DBP-K<sub>2</sub>-CO<sub>2</sub>-CO<sub>2</sub> (TS2); E=-2476.07827976H</p> 	<p>50  C,4.2279690335,-2.7568537161,1.1341446647  C,3.8873793108,-1.4635545037,1.5362554129  C,3.342963306,-0.5577791683,0.6337363012  C,3.1579921492,-0.9809310188,-0.6916904546  C,3.5127538981,-2.2534812805,-1.1117422524  C,4.0463162175,-3.1500572508,-0.1855511547  C,2.4089205612,0.0073938634,-1.5628081647  C,1.0635378565,0.2427682035,-0.8638026789  C,1.1863067918,0.7602189877,0.4436267666  C,0.0129654921,0.9703585593,1.1518676786  H,0.0744231417,1.3951203281,2.150434939  C,-1.2562984064,0.6144594583,0.6438464797  C,-1.3196954877,0.0057294213,-0.6226619716  C,-0.1546394954,-0.1247190803,-1.3956898616  H,4.646970625,-3.4544316803,1.8488191459  H,4.0455788807,-1.16552822,2.5673639895  H,3.3622370707,-2.5562441505,-2.1418774034  H,4.322048209,-4.1489452903,-0.498346009  H,2.2945047405,-0.3089645601,-2.59615794  H,-0.2162161023,-0.5857905272,-2.3747810571  B,2.7503389402,0.9293350537,0.8890135357  C,3.0619543671,1.656783096,2.2754660363  H,2.6479156785,1.0972363701,3.1197025312  H,2.6301115336,2.6629517971,2.3341831034  H,4.1355579259,1.7598750669,2.4507474894  C,3.0345763403,1.3922470238,-1.4993040037  O,3.3353682744,1.7925015914,-0.2910565827  O,3.057039768,2.1501569658,-2.4542800153  C,-3.8442149076,-0.0989648107,-0.579963008  C,-3.893923757,0.6348927929,0.6172196408  C,-5.0194686968,-0.3589266468,-1.2803684852  C,-5.1397087759,1.1012488616,1.0637494776  C,-6.2333395331,0.1237628068,-0.8263822049  H,-7.1371657409,-0.0821473162,-1.3864424978  C,-6.2992744875,0.8639160924,0.3517016902  H,-7.2508056428,1.2366131779,0.708450169  H,-5.1922948428,1.6626787227,1.9901235017  H,-4.9779681326,-0.9567925298,-2.183121867  K,1.3815040414,3.5158402855,-0.7646760132  C,-2.6224740971,1.504351441,2.8617850728  H,-2.8827954502,2.5680049986,2.8002090552  H,-1.685064236,1.4351491681,3.4130971052  H,-3.4059979352,1.043414897,3.4668096377  C,-2.561108188,-0.6787051837,-1.0783279544  H,-2.5735922238,-0.750291408,-2.1682959354</p>

	<p>B,-2.5901131462,0.8974356399,1.4077840851  K,0.7171506789,-2.4413165709,0.581560347  C,-2.4012348303,-2.2268100659,-0.5889347552  O,-1.2740438772,-2.7198066692,-0.8540577964  O,-3.3561732802,-2.7217295927,-0.0190258889</p>
<p>cis-DBP-K<sub>2</sub>-(CO<sub>2</sub>)<sub>2</sub>; E=-2476.10879092H</p> 	<p>50  C,0.104300975,-0.4454732752,-1.5632645352  C,1.2644293293,-0.1596563935,-0.8490090436  C,1.2930346067,-0.1701786348,0.5539854372  C,3.8881746437,-0.0848687933,0.4246096127  C,3.7677511397,-0.0887843329,-0.9684064262  C,4.7605306803,-0.6010977644,-1.7876550524  H,4.6501394638,-0.5818365909,-2.86630365  C,5.9035905145,-1.1432790105,-1.207893385  C,6.0402204616,-1.1575643709,0.1734277863  C,5.0384853966,-0.6269771526,0.982846992  H,0.0890712712,-0.3789256066,-2.6469975144  H,6.6866507934,-1.5498844929,-1.8353865079  H,6.9340939145,-1.5758798457,0.6199681162  H,5.1622049473,-0.6305842944,2.0607559889  C,-3.2342397006,0.5768860347,0.4537539956  C,-3.1458051865,0.5295232167,-0.9466191477  C,-3.5197501661,1.60290245,-1.7386742401  H,-3.4441853459,1.5443441459,-2.8187209048  C,-3.9784743763,2.7718217472,-1.1288295486  H,-4.2676151083,3.6196431394,-1.7365442232  C,-4.0697935369,2.8422255748,0.2545521387  H,-4.4334747543,3.7482645897,0.7234855373  C,-3.7076204996,1.7441944716,1.0395505801  H,-3.7928991208,1.8076616214,2.1194227451  C,-1.0818681358,-0.7238548223,0.5554389135  C,0.121429804,-0.5077182157,1.234517276  H,0.1195465551,-0.4874420628,2.3225169902  C,-1.0622160521,-0.6932268202,-0.8481956948  C,-2.8050208494,-0.9613053544,2.7182462659  H,-2.3495045998,-0.1478827847,3.2907751259  H,-3.8614203498,-0.9998227707,2.9950495912  H,-2.3437910849,-1.8858346481,3.0857555013  B,-2.609499388,-0.7492826633,1.1475889309  C,-2.458321938,-0.7116808393,-1.4852920398  H,-2.4261707775,-0.7650645,-2.5704483478  C,-3.0509290565,-1.9872486389,-0.9121368448  O,-3.2646328724,-1.949247202,0.3785866525  O,-3.120041319,-3.0275161365,-1.5444113082  C,2.6681133445,0.8644743689,2.714173472  H,1.7816606309,1.3938656591,3.0790923224  H,2.7324367744,-0.0732709759,3.275454123  H,3.537835751,1.4654519052,2.991225788  H,2.4153665089,0.5483727334,-2.57109518  C,2.4809565643,0.5071229204,-1.4865424652  B,2.6177743324,0.5904421948,1.1424526894  K,-1.3204520243,-3.7232912948,0.4325448983  K,-0.4912958183,2.323981068,-0.0756101811  O,2.4314563135,1.982137207,0.3850452373  C,2.2645328451,1.9115521641,-0.9019432881  O,1.7721753892,2.8157381057,-1.5613153592</p>
<b><i>trans</i>-Diborapentacene<sup>(2-)</sup>:2K<sup>+</sup></b>	
trans-DBP-K <sub>2</sub> ; E= -2098.81621979H	44



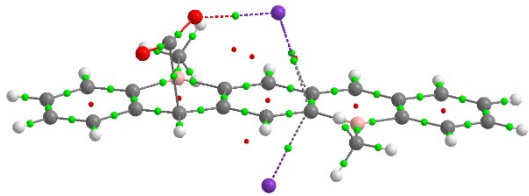
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 C,3.8335602948,0.535803231,-0.0451688278  
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 C,4.8556490141,-1.7220062684,-0.0591369042  
 H,0.0474559113,2.4697522522,0.0480786473  
 H,2.3437880101,-2.582195419,-0.1714877609  
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 H,4.7356161467,-2.7990842475,-0.1106855115  
 B,2.6085555762,1.4327595461,-0.1054847461  
 C,2.6587735437,3.0253015847,-0.1199115927  
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 C,-3.6909907412,0.9052919247,0.0933998462  
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 C,-1.2619389969,-0.69963032,0.0672576221  
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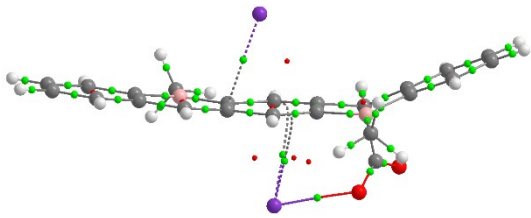
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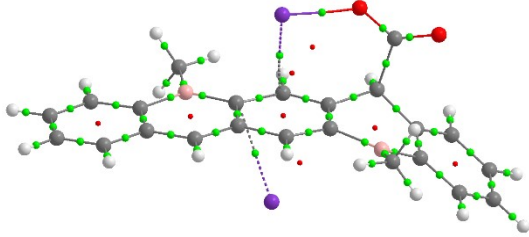


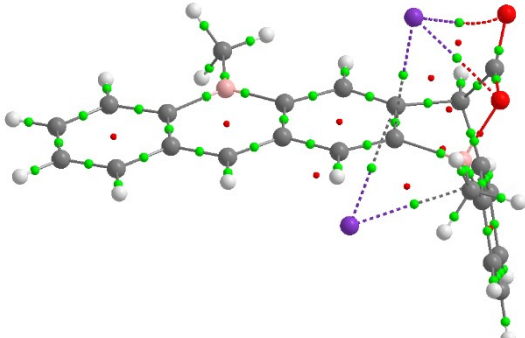
47  
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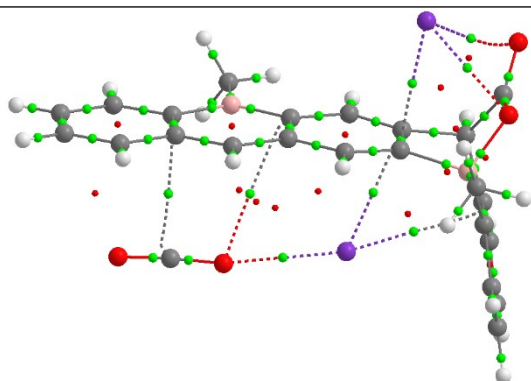


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<p>trans-DBP-K<sub>2</sub>/CO<sub>2</sub> (TS1); E= -2287.41432541H</p> 	<p>47  C,6.0982274014,0.9604106401,-0.0273237078  C,4.9517920921,1.2445161429,0.6598226542  C,3.6649917994,0.8208609767,0.2256573731  C,3.6008056392,0.0607585314,-0.9944818925  C,4.81551493,-0.220902923,-1.6934668879  C,6.0194572513,0.2122500922,-1.2277105115  C,2.3816072637,-0.4072056182,-1.5087045974  C,1.1547727892,-0.1691102359,-0.8682332222  C,1.0935489261,0.5828318725,0.3772888663  C,-0.1711264143,0.7508057303,0.98081317  H,-0.2202098229,1.3146489079,1.9100514816  C,-1.3688898214,0.2284951936,0.471866514  C,-1.3088772816,-0.5029228582,-0.780579466  C,-0.0707858849,-0.6648296043,-1.3971874704  H,7.059705879,1.3010495736,0.3345016695  H,5.0222440586,1.818293026,1.5764078595  H,4.7605528977,-0.7929140309,-2.6134054635  H,6.9249170157,-0.0152103394,-1.7777603665  H,2.3838528287,-0.9718026102,-2.4354647525  H,-0.025751658,-1.2163794976,-2.3337224886  B,2.3925762226,1.1371090261,0.9943341935  C,2.3361112211,1.9641596482,2.3561546651  H,1.6742353825,2.8327182016,2.2724269419  H,1.9239372589,1.3631270873,3.1744028839  H,3.3030127816,2.335174743,2.6948334169</p>

	<p>K,-0.3021088192,2.2842081812,-1.59450622  C,-3.8631051854,-0.9701606416,-0.5156266446  C,-3.8041049498,-0.2265993493,0.7079676325  C,-5.1029562957,-1.561071308,-0.8692509821  H,-5.1626491589,-2.1227273851,-1.7940652142  C,-4.979923941,-0.1322312587,1.5054182796  H,-4.9362214641,0.4354298123,2.4273383029  C,-6.221816981,-1.456617201,-0.0869414941  H,-7.1524329606,-1.9224621736,-0.3831521002  C,-6.1466870084,-0.7278446373,1.1195269606  H,-7.0260479085,-0.6384261927,1.7464891856  K,0.3952204302,-2.1250001102,1.1123299039  C,-3.3169288656,2.4839555859,0.3232704915  O,-4.0781462618,2.8210307692,1.1406288871  O,-2.6777946822,2.6101391817,-0.6698905335  B,-2.6154420014,-1.1143732166,-1.372289325  C,-2.6214589633,0.4375955006,1.1262616194  C,-2.5627719007,-1.8646902067,-2.7706108471  H,-3.5331745532,-2.1902179274,-3.142476189  H,-2.1167048142,-1.2309981029,-3.5440732726  H,-1.9246200028,-2.7538925822,-2.7176874957  H,-2.5987404681,0.8485145868,2.1298341924</p>
<p>trans-DBP-K<sub>2</sub>-CO<sub>2</sub> (inte1); E= -2287.43376572H</p> 	<p>47  C,5.9998508196,0.0451046376,1.0813258377  C,4.7826127983,-0.2103374351,1.6443081995  C,3.5740562893,0.1077015152,0.9620531536  C,3.644267557,0.7094688628,-0.3328897022  C,4.9339595937,0.9521103943,-0.8708183378  C,6.0844464524,0.6353110654,-0.1987898795  C,1.0627156796,0.6835339799,-0.3935472307  C,1.1172205156,0.0928036279,0.9337741387  C,-0.1253445814,-0.2823036441,1.551099204  H,-0.0803208453,-0.6968215304,2.5551599754  C,-1.3432336771,-0.1795619738,0.9183491368  C,-1.3947440032,0.3661855119,-0.4154668479  C,-0.2253337532,0.7919156434,-1.0012768154  H,6.9070402151,-0.2034271009,1.6187199054  H,4.7210243126,-0.6617254403,2.6285526868  H,5.0041495937,1.4094456063,-1.8517550256  H,7.053663752,0.8365390821,-0.6367174072  H,-0.285821057,1.2433783129,-1.9880511566  K,-0.5312773409,2.7736311564,1.2740646411  C,-3.8188512279,-0.3086068042,-0.6786619296  C,-3.844374978,-0.9221070415,0.5876835348  C,-4.8829750469,-0.4985252913,-1.5615748027  H,-4.8765649438,0.0192184493,-2.5127789616  C,-4.9435390244,-1.7294425135,0.9188240997  H,-4.9790700699,-2.1972709289,1.8967527414  C,-5.9459978269,-1.3129179008,-1.2147887348  H,-6.7624097558,-1.4548992335,-1.9121709891  C,-5.9794942701,-1.9398048607,0.0295072429  H,-6.8165321146,-2.5709416409,0.2988058248  K,0.5189681257,-2.07177877,-0.7822645548  B,-2.6758266743,-0.6774642619,1.5713516642  C,-2.8024266486,-1.0156764152,3.1026853424  H,-2.8787943222,-2.1009842711,3.2371969651  H,-1.9752889647,-0.6689246569,3.7219463457  H,-3.7287904938,-0.6034042678,3.509644705  C,-2.7222395142,0.6434922666,-1.0484075096</p>

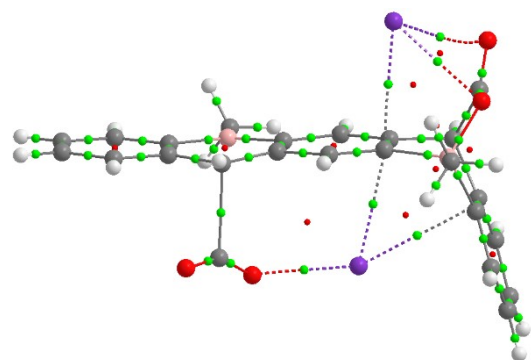
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<p>trans-DBP-K<sub>2</sub>/CO<sub>2</sub> (TS2); E= -2287.42973715H</p> 	<p>47  C,5.6461761576,-1.6180436129,0.3424648182  C,4.5807438326,-1.308114199,1.1704484109  C,3.5340851168,-0.4840412974,0.7383555814  C,3.588894651,0.0481534872,-0.5662251984  C,4.67649633,-0.2432039159,-1.381488524  C,5.6919798179,-1.0757401288,-0.9368600846  C,2.5233445188,0.9961578292,-1.0355359608  C,1.1581303617,0.6234028968,-0.5466829997  C,1.0259453978,0.2577012347,0.8457238417  C,-0.233868867,0.0915989883,1.3700238621  H,-0.3463940094,-0.1822835027,2.4158586493  C,-1.4334828758,0.197813096,0.5823576813  C,-1.2991368046,0.5429099747,-0.8234247859  C,0.0296546048,0.7578552654,-1.3124528153  H,6.4436716418,-2.2613805037,0.6910870369  H,4.557969036,-1.713329432,2.1757203533  H,4.734243077,0.2005651994,-2.3682948383  H,6.5300135259,-1.2953307521,-1.5868957696  H,2.5243518806,1.0542303077,-2.1266694953  H,0.1504417289,1.0619666189,-2.3479923317  B,2.3266846805,-0.1113712523,1.6405766544  C,2.3975879437,-0.1271636111,3.2051844233  H,3.0278263425,-0.9212817981,3.6086673122  H,1.4348613174,-0.1478208706,3.7163690702  H,2.8891082754,0.8117973344,3.4911298588  C,2.8417715018,2.4912786942,-0.5439898043  O,3.9696675387,2.7117437165,-0.1345581313  O,1.8563134719,3.2725182102,-0.6415669344  C,-3.8621711856,0.2827598099,-0.9828029009  C,-3.8700704751,-0.0528904002,0.4064994151  C,-5.1083909902,0.2859508072,-1.6593426671  C,-5.1075743727,-0.3604965837,1.0392250027  C,-6.2882383708,-0.0148799701,-1.0319612679  H,-7.2230080874,-0.0013353403,-1.5776973052  C,-6.2810283914,-0.3420922542,0.34158892  H,-7.2121817949,-0.5779168582,0.8423648359  H,-5.1042456694,-0.6104846066,2.0945643237  H,-5.1207281329,0.5387956357,-2.7139793035  K,-0.3795658907,3.1973201973,0.3007548062  K,-0.189569281,-2.090733376,-0.6992339222  B,-2.5486413837,0.6179752818,-1.6956347299  C,-2.5250838643,0.9923486535,-3.2446150469  H,-2.92657585,0.1767095848,-3.8548366678  H,-3.1698903775,1.852674615,-3.4489441021  H,-1.5394119827,1.234285416,-3.6444930457  C,-2.6708457209,-0.0875668276,1.1525985802  H,-2.7164842028,-0.3425924812,2.2063669952</p>

<p>trans-DBP-K<sub>2</sub>-CO<sub>2</sub> ; E= -2287.47130843H</p> 	<p>47</p> <p>C,-3.5536916279,-3.391291068,-0.429590968  C,-3.465019911,-2.2244673197,-1.1923053015  C,-3.2599998635,-0.9884863628,-0.5880319487  C,-3.1563456816,-0.9490195764,0.8130925687  C,-3.2610750237,-2.0978943393,1.5838008886  C,-3.4545755147,-3.3284101038,0.9548530113  C,-2.7279513153,0.3930115577,1.3661410881  C,-1.360889089,0.6658987986,0.7225935438  C,-1.403161607,0.6875538135,-0.7163142067  C,-0.2245328961,0.7779802253,-1.3995964911  H,-0.2326341844,0.787901972,-2.4881752408  C,1.0607540994,0.7645585458,-0.7347419456  C,1.0839141866,0.7527879742,0.7201510029  C,-0.166167445,0.7304190937,1.3944389592  H,-3.7139322111,-4.3466867364,-0.9141604708  H,-3.5513495207,-2.2846241788,-2.2724434548  H,-3.1805356409,-2.0438072337,2.6640343316  H,-3.5375805562,-4.2309117436,1.547148851  H,-2.6941211204,0.4348797558,2.4520702428  H,-0.1680474269,0.7081986557,2.4809489721  B,-2.9203262131,0.4428220297,-1.2725555169  C,-3.1892391479,0.622409127,-2.8362813528  H,-2.6025998118,-0.0872018457,-3.4280450115  H,-2.9185332085,1.6213763806,-3.195156385  H,-4.2402658674,0.4639447175,-3.0905476772  C,-3.5577934448,1.5418745699,0.8221532468  O,-3.7462805007,1.5046635163,-0.4727633012  O,-3.8264958367,2.530815744,1.4843830524  C,3.659933982,0.6203286776,0.545132665  C,3.5106020266,0.6302408488,-0.8739333733  C,4.9735843072,0.5379261372,1.0649770136  C,4.6722122869,0.558130632,-1.6894615231  C,6.0831588151,0.4681545102,0.2611274754  H,7.074993756,0.4070730437,0.6907307796  C,5.9216366033,0.4793877776,-1.1389544609  H,6.7928486146,0.4267218975,-1.7810536115  H,4.5523329841,0.5682276014,-2.7675091285  H,5.1019675738,0.5316404097,2.1422644959  K,-1.9115332814,3.5118841446,-0.251738572  K,-0.2782198983,-1.9216508199,-0.0664839603  B,2.4245638547,0.7005984051,1.4498529278  C,2.5722945077,0.70736425,3.0368058182  H,3.0860682574,-0.1920597533,3.3910343788  H,3.1939806393,1.547908466,3.3605029107  H,1.6337961237,0.7785025065,3.5889371527  C,2.2294533114,0.7064746505,-1.4753702967  H,2.1651239159,0.7206376459,-2.5587301784</p>
<p>trans-DBP-K<sub>2</sub>-CO<sub>2</sub>:CO<sub>2</sub>; E= -2476.08344116H</p>	<p>50</p> <p>C,4.7577425904,-1.5976599477,0.2762338711  C,4.166854398,-0.5949705451,1.048050546  C,3.5265065609,0.4845467332,0.4490565489  C,3.5014883694,0.5397203574,-0.9546595478  C,4.0993828522,-0.4404625191,-1.7331628024  C,4.7265657557,-1.5199269132,-1.1104034794  C,2.6232432862,1.636062715,-1.517365514  C,1.217705178,1.3504832883,-0.9711902934  C,1.1595370465,1.3246938413,0.4658240718  C,-0.0163123533,0.9676496381,1.0615312474</p>

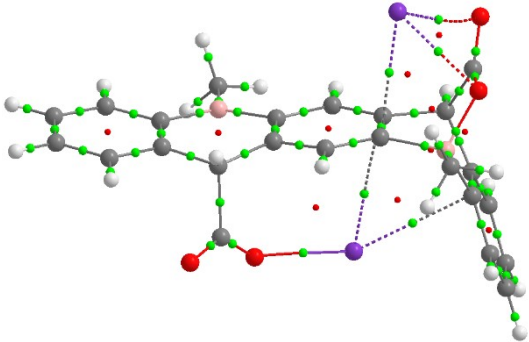


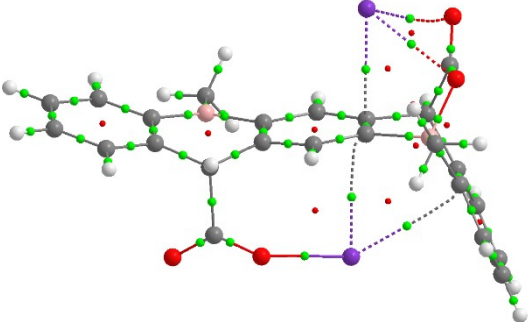
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 H,5.1961856524,-2.2905735941,-1.7085241862  
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 B,2.6187111348,1.6438138367,1.1281493753  
 C,2.6995786945,1.847347912,2.7098242844  
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 O,-1.2119507015,-2.8395354203,-0.4466333381  
 O,-3.3858771138,-3.6156548642,-0.468784208  
 B,-2.2945630544,0.1194480352,-1.97349079  
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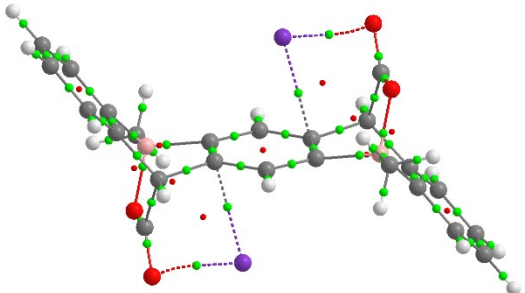
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 H,4.1579210306,-0.3619478317,-2.8183968073  
 H,5.4156539015,-2.2042126825,-1.7307784645

	<p>H,2.5759125214,1.6039706655,-2.5843737776  H,0.1675142226,0.8250623636,-2.8013932723  B,2.5556410884,1.4992944003,1.1434702387  C,2.6142052035,1.6931994877,2.7263381645  H,2.3544159845,0.7694963367,3.2524662587  H,1.9144876564,2.457510851,3.0824726342  H,3.610388273,1.9887887318,3.0644943607  C,2.7718205546,2.8858663468,-0.8661222667  O,2.8862062892,2.8608122968,0.4370916289  O,2.6171507146,3.9276939889,-1.4810453953  C,-3.5703249704,-0.5491499109,-1.1749594643  C,-3.5319080004,-0.5635920722,0.2431725058  C,-4.7812302244,-0.9027360887,-1.8081816803  C,-4.695868063,-0.9187068079,0.9615535817  C,-5.9069604075,-1.2440614608,-1.0978014023  H,-6.8244467652,-1.5076826124,-1.6079001958  C,-5.8549245748,-1.2481966561,0.3052955257  H,-6.736656871,-1.516177495,0.8749194319  H,-4.65634724,-0.9392835606,2.044040862  H,-4.821267668,-0.8987668689,-2.8920207336  K,0.419211462,3.9550427188,0.1880640288  K,1.3875849919,-1.7509532841,-0.3379830051  C,-1.7166556089,-2.2859048943,1.3478062386  O,-0.8654335052,-2.5611752965,0.5520706249  O,-2.3778707227,-2.598992542,2.2681551506  B,-2.325966207,-0.1301458833,-1.9700146148  C,-2.3293639441,-0.1491743771,-3.5561076335  H,-2.6355141628,-1.1305319374,-3.9298538825  H,-3.0723785015,0.5569768256,-3.9406565846  H,-1.3793569856,0.09705148,-4.0311296144  C,-2.3191528595,-0.2581747101,0.9576288506  H,-2.4092095961,-0.0601559856,2.0197524542</p>
<p>trans-DBP-K<sub>2</sub>-CO<sub>2</sub>-CO<sub>2</sub> (inte1);  E= -2476.0832307H</p> 	<p>50  C,-4.1210314436,-3.0222400261,0.2534098326  C,-3.7346806986,-2.1126747515,-0.7330697279  C,-3.2841337481,-0.8431207125,-0.3916142877  C,-3.2445270877,-0.4983377526,0.9684022511  C,-3.6425586109,-1.3846208607,1.9568110302  C,-4.0765921863,-2.6595660064,1.5932008799  C,-2.5990622305,0.8430366969,1.2551415608  C,-1.1802661553,0.7578826428,0.6790491792  C,-1.1482152292,0.4697100191,-0.7033932702  C,0.0867495424,0.2529177132,-1.2891123047  H,0.1436722596,-0.0157297742,-2.3417510647  C,1.2771245841,0.267164555,-0.5365797381  C,1.2364423988,0.5971514849,0.8287610488  C,-0.0198615158,0.8540073108,1.4178314257  H,-4.4657985979,-4.0104704693,-0.0246188673  H,-3.7799419194,-2.4041528466,-1.7771494215  H,-3.6074357884,-1.0972164375,3.0017491983  H,-4.3852708219,-3.3625369958,2.3563043028  H,-2.6099838715,1.1262723285,2.3045060271  H,-0.0763620692,1.0931554102,2.4747426776  B,-2.652394627,0.3126930999,-1.3331107389  C,-2.7900744981,0.1830138269,-2.9173592381  H,-2.2929796908,-0.7179166881,-3.2890241906  H,-2.3362870732,1.0242446639,-3.4546106559  H,-3.8350043927,0.1297446116,-3.2322252805  C,-3.1989634588,1.9510151602,0.4046109026</p>

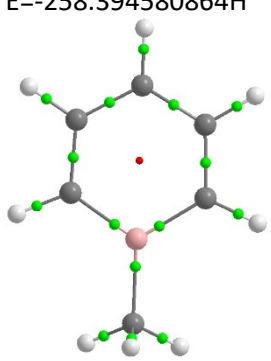
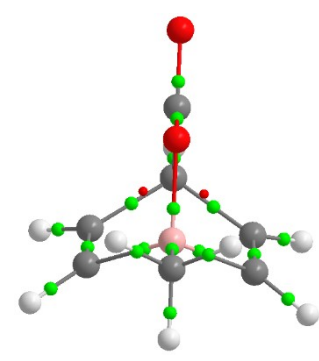
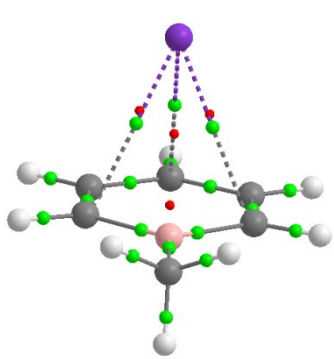
	<p>O,-3.348960019,1.6377900558,-0.8575778656  O,-3.3224458138,3.0972767493,0.8010601902  C,3.8707359635,0.4432230601,0.8366250885  C,3.8114398014,0.0462781627,-0.5105683338  C,5.1353001865,0.6524658226,1.4144981464  C,4.9930695941,-0.144421719,-1.2329748198  C,6.2985570783,0.483420654,0.6930168103  H,7.2625978795,0.6547655394,1.1544706616  C,6.2201311817,0.0768194512,-0.6392346104  H,7.1271841425,-0.0723620204,-1.2120458121  H,4.9292813645,-0.49367604,-2.2556131179  H,5.1958033723,0.9575394003,2.4531628916  K,-1.4502965383,3.4372274837,-1.1904272967  K,-0.6264388881,-2.3331262853,0.4324594901  C,2.391700357,-1.8563918318,-1.3396959604  O,1.6190026078,-2.4079727753,-0.517466481  O,3.0681140789,-2.3339778898,-2.2327067608  B,2.5677248324,0.6460365385,1.6410459412  C,2.6079802411,0.9454100671,3.1886743949  H,3.3063384873,0.279996516,3.7012690863  H,2.9944184659,1.9588999567,3.3473387653  H,1.6494769346,0.8844945272,3.7031339659  C,2.5105542337,-0.2418726697,-1.1908051698  H,2.5563143862,0.0963330439,-2.2267827346</p>
<p>trans-DBP-K<sub>2</sub>-CO<sub>2</sub>/CO<sub>2</sub> (TS2);  E= -2476.07911819H</p> 	<p>50  C,-4.3559507564,-2.9432725605,0.1040519354  C,-3.8918806084,-2.0160233819,-0.8309338152  C,-3.3338163504,-0.8110319099,-0.4196849836  C,-3.2697569325,-0.544981714,0.9566965581  C,-3.7421483442,-1.4496892975,1.8945453228  C,-4.2802322557,-2.6614152726,1.4619020471  C,-2.5414308791,0.7343879078,1.3154869113  C,-1.1249429143,0.6122426394,0.7423896551  C,-1.1000733151,0.3629755711,-0.6472887896  C,0.1270017062,0.1278599601,-1.2434637477  H,0.1765544818,-0.1273860349,-2.2976375424  C,1.318152608,0.1271564081,-0.4942135627  C,1.293925089,0.4954542084,0.8621381685  C,0.0430607216,0.7284666323,1.4694847886  H,-4.7867075752,-3.8800946693,-0.2272598087  H,-3.9633563644,-2.2409995958,-1.8902149495  H,-3.6861805981,-1.225113798,2.9537643416  H,-4.6467984442,-3.3776319827,2.1860449719  H,-2.546158037,0.9655141313,2.3775147799  H,0.0012768454,0.975592596,2.5263563996  B,-2.6047593018,0.3367072348,-1.2948263449  C,-2.7274087579,0.2912378398,-2.8850006674  H,-2.2881735179,-0.6243558912,-3.2931223978  H,-2.2075883063,1.1231648426,-3.3738480203  H,-3.7684726326,0.3263425583,-3.2149883895  C,-3.061830634,1.9223814159,0.5175615836  O,-3.2038218524,1.6883697808,-0.762101574  O,-3.1208386606,3.0494510473,0.9784546702  C,3.9261239544,0.5725526378,0.7720681118  C,3.8446766636,0.0701714868,-0.5396517579  C,5.1788713487,0.9827507761,1.2521075511  C,4.99696237,-0.0261619005,-1.3147759969  C,6.3146578112,0.9112978062,0.4683808336  H,7.2712018103,1.2387621423,0.8547076107</p>

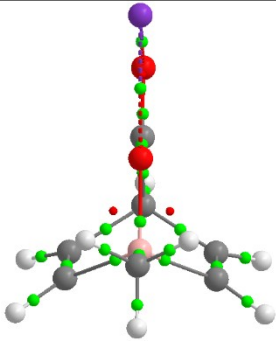
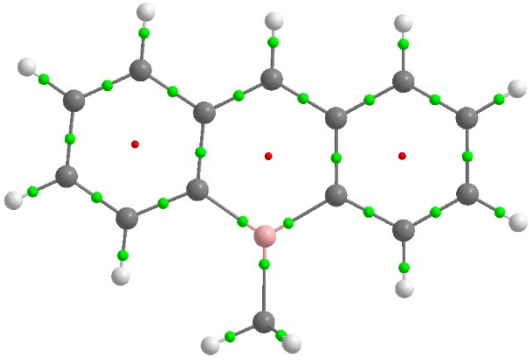
	<p>C,6.218414507,0.3967195428,-0.8215288177  H,7.1038346907,0.320006927,-1.4405593693  H,4.932735886,-0.4492658782,-2.3103581087  H,5.2583721035,1.3695721405,2.2612169137  K,-1.0820328802,3.3235187309,-0.8742434807  K,-0.8027094501,-2.5742474002,0.027740608  C,2.4291044054,-2.0515951488,-0.875510419  O,1.3124697514,-2.5142268824,-1.225291588  O,3.3943509761,-2.6147560328,-0.3948695216  B,2.6447640493,0.6553900969,1.6330537468  C,2.6412612733,0.9595790821,3.1784260458  H,2.0103402854,0.245295411,3.715232302  H,3.6253169108,0.9466399079,3.6436917018  H,2.1999242238,1.9448550698,3.3677769758  C,2.5553390434,-0.438952288,-1.0963095415  H,2.5352033025,-0.3233045629,-2.1822970707</p>
<p>trans-DBP-K<sub>2</sub>-(CO<sub>2</sub>)<sub>2</sub> ; E= -2476.10879089H</p> 	<p>50  C,0,-0.007576,0.03725,1.399088  C,0,-1.194944,0.287317,0.708679  C,0,-1.166027,0.23225,-0.695688  C,0,-3.633653,-0.102227,-0.79175  C,0,-3.750502,-0.044786,0.601624  C,0,-4.779277,-0.76015,1.201081  H,0,-4.899973,-0.727007,2.278746  C,0,-5.665478,-1.511737,0.43212  C,0,-5.535619,-1.548296,-0.949451  C,0,-4.514467,-0.834946,-1.571236  H,0,0.002675,0.065883,2.485968  H,0,-6.466004,-2.062636,0.910404  H,0,-6.231578,-2.125128,-1.545247  H,0,-4.413733,-0.851062,-2.650914  B,0,-2.612882,0.879245,1.269766  C,0,-2.699669,1.219766,2.825945  H,0,-3.648292,1.696987,3.083353  H,0,-2.62002,0.313231,3.434354  H,0,-1.901497,1.893228,3.156535  C,0,3.753616,0.041809,-0.601793  C,0,3.636661,0.099323,0.791529  C,0,4.51984,0.828807,1.571382  H,0,4.418913,0.845011,2.651041  C,0,5.543573,1.538752,0.949993  H,0,6.2414,2.113054,1.546051  C,0,5.673598,1.502075,-0.431571  H,0,6.476123,2.050331,-0.909544  C,0,4.784987,0.753747,-1.200881  H,0,4.905774,0.720456,-2.278529  C,0,1.196646,-0.283058,-0.709399  C,0,0.009383,-0.032451,-1.399807  H,0,-0.000928,-0.061317,-2.486678  C,0,1.167713,-0.228152,0.694962  C,0,2.699424,-1.218869,-2.826626  H,0,2.622393,-0.311998,-3.434874  H,0,3.6468,-1.698625,-3.083922  H,0,1.899486,-1.890109,-3.157414  B,0,2.613309,-0.878319,-1.270445  C,0,-2.470417,0.681201,-1.354311  H,0,-2.412579,0.674726,-2.439983  C,0,-2.494476,2.126035,-0.845505  O,0,-2.157996,3.064781,-1.551037</p>

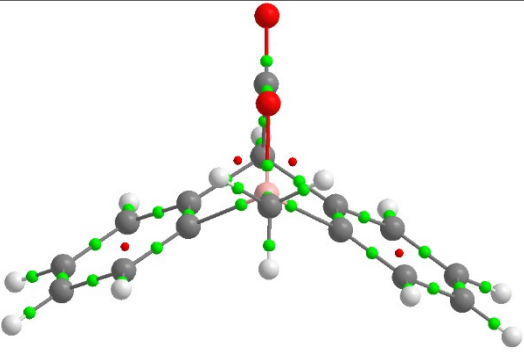
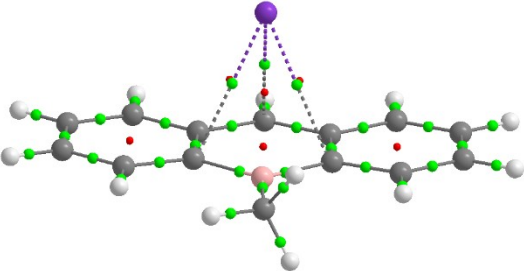


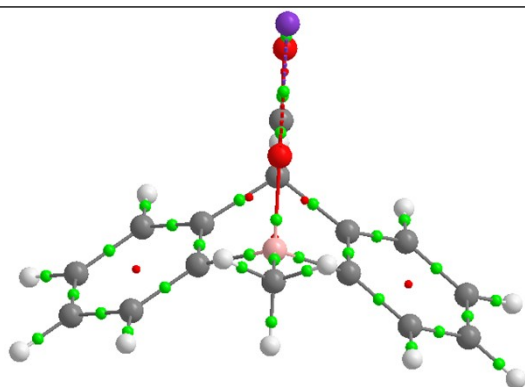
	O,0,-2.662276,2.235302,0.440846
	C,0,2.470857,-0.680454,1.353688
	H,0,2.412828,-0.674078,2.439353
	C,0,2.490437,-2.125354,0.84453
	O,0,2.658231,-2.234922,-0.441672
	O,0,2.150508,-3.063036,1.54994
	K,0,-0.10476,-2.898747,0.015187
	K,0,0.096894,2.906131,-0.013058

**MONOMERS AND ADDUCTS IN THF**

<b>BBZN<sup>(-)</sup></b>	
BBZN (THF) ; E=-258.394580864H 	15 C,0.6522584247,-1.124079898,-0.8321457005 C,0.7099089499,0.1368762915,-1.4199670905 C,-0.3277673528,1.0673900426,-1.2964408059 C,-1.4767152515,0.7473696606,-0.5647351989 C,-1.6391514678,-0.4843308697,0.0640697573 H,-0.2431623284,2.0379608463,-1.7729526218 B,-0.5564689494,-1.5405827295,-0.0195204626 C,-0.6692729821,-2.9688291246,0.7116028735 H,-0.2599378456,-2.9274213315,1.7283773982 H,-1.7036236856,-3.313952612,0.8141999519 H,-0.1145089872,-3.7576983094,0.1925265744 H,1.5157755408,-1.7715320098,-0.9968788595 H,1.5824146541,0.4277535318,-2.0035182397 H,-2.2607418458,1.5007412856,-0.5003842172 H,-2.5770641355,-0.6288370377,0.6039131737
BBZN-CO <sub>2</sub> (THF) ; E=-446.994729411H 	18 C,-0.6964680058,1.2946312425,0.6356183744 C,-0.8601111706,1.2532083231,-0.6842935181 C,-0.3031759261,0.0007397135,-1.3599389863 C,-0.8657737266,-1.2492673987,-0.6844309827 C,-0.7023212803,-1.2915696106,0.6354766004 H,-0.4198960127,0.0010626361,-2.4393874836 C,0.5985489225,-0.0015179155,2.7225588901 H,-0.2678601155,0.0004061839,3.3941146779 H,1.1960511589,-0.8845540618,2.9758640515 H,1.2000409033,0.8787780334,2.9759594324 O,1.4142288685,-0.003223321,0.2755415237 C,1.1905890243,-0.0026687953,-1.0060403593 O,2.0692854091,-0.0045640938,-1.8514103922 B,0.1351689874,-0.0003866023,1.1842074931 H,-1.0631259156,2.1369968403,1.2196495151 H,-1.3203496558,2.0148364693,-1.3065395437 H,-1.3294561324,-2.0087365634,-1.3067591713 H,-1.0727931982,-2.1323273516,1.2194175012
<b>BBZN<sup>(-)</sup>:K<sup>(+)</sup></b>	
BBZN-K (THF); E=-858.267050358H 	16 C,0.558868251,-0.903167624,-0.4438799458 C,0.5717826857,0.3414339396,-1.0722793086 C,-0.5908204927,1.108579261,-1.2328820484 C,-1.8238927878,0.6270802624,-0.7705409759 C,-1.9462044316,-0.6044455311,-0.1283943237 H,-0.5395941484,2.0679377624,-1.7344002929 B,-0.7389566187,-1.5040843427,0.0644028305 C,-0.8251246563,-2.9484220754,0.7497803674 H,-1.6362442864,-3.0300188893,1.480390162 H,-1.0179593122,-3.7213337364,-0.0035934379 H,0.1016088558,-3.2416954895,1.2532318215 K,-0.2264457889,1.0364795238,1.7278559995 H,1.5199210377,-1.413323357,-0.3714944623 H,1.5046200344,0.7514471058,-1.4542183681 H,-2.7007135881,1.2528918214,-0.924550698 H,-2.9515406956,-0.8801350054,0.1916437668
BBZN-K-CO <sub>2</sub> (THF) ; E=-1046.86493537H	19 C,-0.7017507509,1.2942830445,0.6355737667

	<p>C,-0.8616777055,1.2563420576,-0.6838037213  C,-0.3096070323,0.000775897,-1.366151361  C,-0.8674029701,-1.2523347899,-0.6839212858  C,-0.7074888859,-1.2912400099,0.6354305058  H,-0.4299701646,0.0011039858,-2.4446071737  C,0.5981697479,-0.0015013608,2.7235483452  H,-0.2623807991,0.0003815233,3.4014891321  H,1.1931223594,-0.8865774861,2.9748206491  H,1.1970665475,0.8808827496,2.9749171761  O,1.4058982892,-0.0031846929,0.2684196071  C,1.1675029544,-0.0025813389,-1.0145619902  O,2.0772162245,-0.0046345974,-1.8398187056  B,0.1096553191,-0.000324162,1.1981031227  K,3.9911462508,-0.0089089709,-0.0229521134  H,-1.0717349183,2.1332178646,1.2207055715  H,-1.3194566696,2.0171372314,-1.3070985485  H,-1.3286383577,-2.010973624,-1.3072955094  H,-1.0811819582,-2.1285993911,1.2204624424</p>
<b>BA<sup>(-)</sup></b>	
<p>BA (THF) ; E=-754.321183894H</p> 	<p>27  C,-7.7667226634,-1.8420359559,0.0144873295  C,-6.3947208286,-1.8761181155,0.0087619099  C,-5.592073471,-0.7062014686,-0.0009897188  C,-6.2687368406,0.5619180193,-0.0048999112  C,-7.699339199,0.5717002165,0.0012151695  C,-8.4223190777,-0.5867996644,0.010561756  C,-5.5512929863,1.7681622403,-0.0144829375  C,-4.1500593679,1.8103294184,-0.0207411305  C,-3.3598321539,0.6049849215,-0.0176594159  C,-1.947354165,0.7547471303,-0.0245400847  H,-1.3343181394,-0.1407302948,-0.0223689271  C,-1.3216861629,1.9753399544,-0.0337956896  C,-2.1099389914,3.1525904824,-0.036731577  C,-3.4719957256,3.0714648005,-0.0304348874  H,-8.3466871858,-2.7569754202,0.0219042781  H,-5.8956966693,-2.8410546647,0.0117970492  H,-8.2102208287,1.5297099242,-0.0017336171  H,-9.5060199055,-0.5468527827,0.015018134  H,-6.1019419688,2.7041144455,-0.0171431328  H,-0.2407539759,2.0460423606,-0.0388287234  H,-1.6264987291,4.1233103814,-0.0440277188  H,-4.0693932306,3.9780274111,-0.0327339069  B,-4.0628511138,-0.7524493899,-0.0073554313  C,-3.2901100819,-2.1522178505,-0.003095438  H,-2.2014720046,-2.0673518928,-0.0078665248  H,-3.5564972569,-2.7509489392,0.8751740512  H,-3.5634410264,-2.7600430568,-0.8729484144</p>
<p>BA-CO<sub>2</sub> (THF) ; E=-754.321183894H</p>	<p>30  C,-7.5334930772,-1.5135835719,-1.0264764082  C,-6.2446862429,-1.7216658005,-0.5300546004  C,-5.5809165733,-0.7236368724,0.1721146027  C,-6.2443384332,0.4978431494,0.3625563772  C,-7.5267451035,0.7162697788,-0.1138542805  C,-8.1737317531,-0.3000866938,-0.8172630118  C,-5.4269305841,1.532885397,1.1200881106  C,-4.1172540152,1.7469545526,0.3769806949  C,-3.3717628545,0.5736579571,0.1871764023  C,-2.169758054,0.6712669556,-0.5022804215</p>

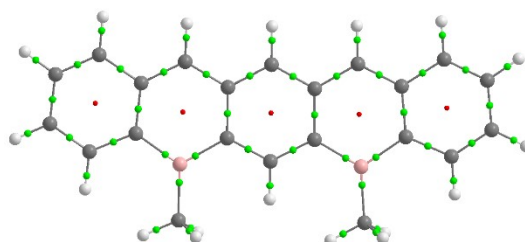
	<p>H,-1.5662513277,-0.2168215042,-0.6664430402  C,-1.7186732199,1.9010709341,-0.9869057146  C,-2.4686772586,3.0501206804,-0.7785095932  C,-3.678527313,2.9760917514,-0.087758123  H,-8.0390830153,-2.3015663871,-1.5727542979  H,-5.7614369206,-2.6803681891,-0.6950717166  H,-8.0219086166,1.6672246847,0.0519071384  H,-9.1745548189,-0.1396214702,-1.1998920616  H,-5.9709639565,2.4572414613,1.2984066604  H,-0.778726407,1.9619468093,-1.5233306362  H,-2.1174345487,4.0045622854,-1.1519670953  H,-4.2694715516,3.8708060651,0.0773184381  C,-3.2942557145,-2.0963447929,0.9002019176  H,-3.0720227143,-2.4630421761,-0.1082383775  H,-2.3355128392,-1.9957694804,1.4209605382  H,-3.8544018704,-2.8877055576,1.4105716946  O,-4.3939601223,-0.2402487068,2.318159087  C,-5.0509863576,0.8774831345,2.4550425793  O,-5.3443249596,1.3635589891,3.5307025364  B,-4.1054561269,-0.7144677629,0.8590343509</p>
<b>BA<sup>(-)</sup>:K<sup>(+)</sup></b>	
<p>BA-K (THF) ; E=-1165.54694992H</p> 	<p>18  C,-3.7379083727,0.368554233,0.0491702169  C,-2.5820399909,1.1023502222,0.0291467066  C,-1.2908750129,0.5058799072,-0.0101024351  C,-1.2258646384,-0.9300686429,-0.0320446825  C,-2.4486682481,-1.6732882194,-0.0087646491  C,-3.6598915998,-1.0461786988,0.0291075779  C,0.0119435934,-1.600086621,-0.0380152473  C,1.2401883992,-0.9154887414,-0.0347829878  C,1.2962871149,0.5247277499,-0.0122149755  C,2.5879465755,1.1236658569,0.0286607203  H,2.6532473211,2.2060045739,0.0418671913  C,3.7463959452,0.3953305017,0.0479853407  C,3.6760579793,-1.0201953763,0.0248810111  C,2.4683795455,-1.6519075351,-0.0137212136  H,-4.7047044887,0.8557447682,0.0756773255  H,-2.645925308,2.1859641037,0.038883806  H,-2.3962008383,-2.7569960463,-0.0276519856  H,-4.5712261734,-1.6329613109,0.0417389296  H,0.018973495,-2.6850777372,-0.0606685071  H,4.7103562804,0.8879416911,0.0761459832  H,4.5902024892,-1.6026418214,0.0360439745  H,2.4204559716,-2.7357722578,-0.0343317588  B,-0.0027373057,1.3339529013,-0.038615515  C,-0.057362608,2.9269263262,-0.0469927993  H,0.9190925984,3.4141164444,-0.0277442044  H,-0.5733119705,3.2903384229,-0.9427475404  H,-0.6270723058,3.3221794028,0.8013138557  K,0.0114611526,-0.3096889169,2.6160697425</p>
<p>BA-K-CO<sub>2</sub> (THF) ; E=-1354.18928999H</p>	<p>31  C,3.3778007365,0.6792993662,-1.3090909274  C,2.3663407243,1.3511103333,-0.6207095264  C,1.2826911687,0.6586111054,-0.0956364653  C,1.2373775731,-0.7298495482,-0.2828510746  C,2.2385852748,-1.4135321526,-0.9521180707  C,3.3159943703,-0.6976352125,-1.4725949623  C,-0.0000933051,-1.3984781079,0.3044397999</p>



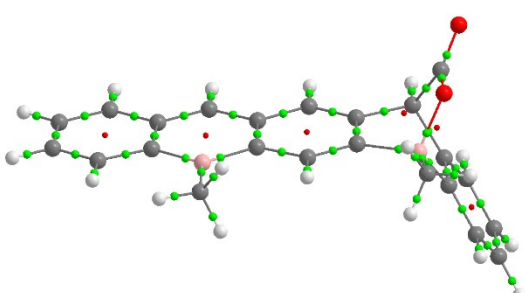
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 C,-2.3662808023,1.3512229279,-0.6210316128  
 H,-2.4324789967,2.4277633261,-0.4958843087  
 C,-3.3777098814,0.6794432505,-1.3094914331  
 C,-3.3159438002,-0.6974951871,-1.4729773239  
 C,-2.2386069165,-1.4134303519,-0.9524029731  
 H,4.2167695031,1.2317549518,-1.7157798203  
 H,2.4325611745,2.4276492055,-0.4955622317  
 H,2.1831371996,-2.4893072564,-1.0780560741  
 H,4.1023607059,-1.2178032306,-2.0058892884  
 H,-0.0001137803,-2.4788294337,0.1855512285  
 H,-4.2166304178,1.2319244213,-1.7162442283  
 H,-4.1022945469,-1.217640979,-2.0063169921  
 H,-2.1831993599,-2.4892115645,-1.0783062852  
 C,-0.0000593877,2.7218894242,1.2320117624  
 H,0.0000453657,3.4123212959,0.3817655443  
 H,-0.8832189129,2.965061301,1.8327970608  
 H,0.8830063152,2.9649998179,1.8329611702  
 O,-0.000207059,0.2525856672,2.0116578269  
 C,-0.0001810615,-1.0332612654,1.7788678325  
 O,-0.0002085639,-1.8521307471,2.6898481228  
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 K,-0.0000774791,-0.0384416552,4.6168425201

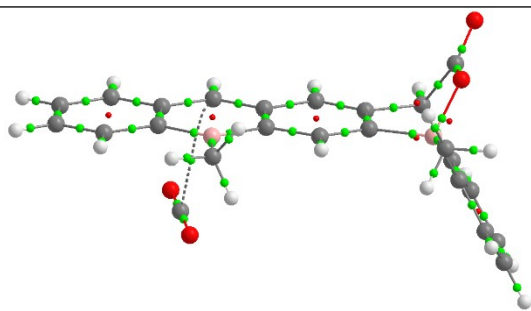
***cis*-DBP<sup>(2-)</sup>**

*cis*-DBP (THF) ; E=-899.106539122H



42  
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 C,1.2918559008,-0.9100372979,0.0004309692  
 C,0.0511685635,-1.5966793572,0.0004188498  
 C,-1.1819144415,-0.9441394229,0.0002777778  
 C,-1.2865869371,0.5001833164,0.0002599853  
 C,-2.5864188585,1.0623291978,-0.0000896154  
 H,-2.6772248611,2.1443884703,-0.0001075191  
 C,-3.7380443646,0.3109852352,-0.000361914  
 C,-3.6259820636,-1.1020750909,-0.0003014074  
 C,-2.4013917425,-1.7038377392,0.000001945  
 H,2.5859926462,2.2426139512,0.000307696  
 H,0.0631478305,-2.683413258,0.0003574737  
 H,-4.7133710882,0.7821823604,-0.0006052528  
 H,-4.5236710098,-1.7115938431,-0.000516897  
 H,-2.3320301934,-2.7876364242,-0.0000000656  
 B,-0.0029375424,1.3317333943,0.0007095848  
 C,0.0116739014,2.9304999917,-0.0001468484  
 H,-0.9779049547,3.3927071459,-0.0005598  
 H,0.5444552308,3.3224595943,0.8734273318  
 H,0.5447302228,3.3215458849,-0.8739743942  
 C,4.9658620782,-1.708643491,0.0000260777  
 H,4.8991949685,-2.7933653382,0.0000464682  
 C,6.2305990279,-1.1171157886,-0.0000868265  
 C,6.3973144547,0.3176228081,-0.0001160906  
 C,7.7166349313,0.8282311153,-0.000155675  
 H,7.8469311476,1.9073888519,-0.0001529381  
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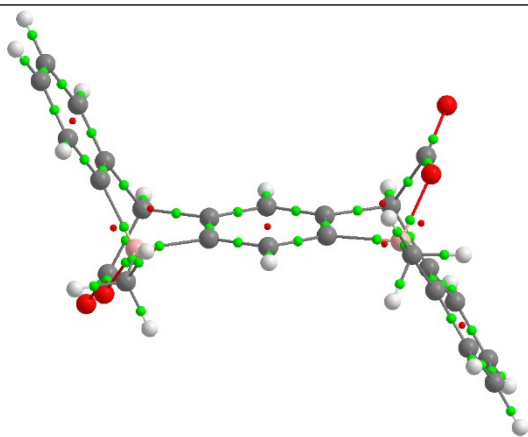
	<p>H,7.3015882012,-3.0078679788,-0.0001607439  C,3.7614753441,-0.9619472724,0.0001577377  C,2.5115764066,-1.6028210741,0.0003002926  H,2.489171057,-2.6909363301,0.0002723353  C,3.8032928249,0.4906680377,0.000127807  C,5.3053295017,2.8066423002,0.00022315  H,5.8673110134,3.1528362797,0.8751115656  H,5.8692783221,3.1531561472,-0.8732508699  H,4.3574396692,3.3484282715,-0.0007159391  B,5.1569681241,1.2141644208,-0.0000533431</p>
<p><i>cis</i>-DBP-CO<sub>2</sub> (THF) ; E=-1087.75498612H</p> 	<p>45  C,0.1580400634,-0.9663568075,0.6543921592  C,1.3058227199,-0.538062815,0.0570208808  C,1.3505200045,0.62911095,-0.7639156016  C,3.7823302541,0.9372332587,-0.013343841  C,3.6424038918,-0.2230871932,0.7656167874  C,4.3422564064,-0.3992810932,1.9484228349  H,4.2183443182,-1.3063008872,2.5309340199  C,5.2009954275,0.6076432452,2.390338404  C,5.3490001205,1.7673677783,1.6423600919  C,4.6440721481,1.9258287347,0.4469387017  H,0.1577727925,-1.862094901,1.2709776682  H,5.7487708177,0.4833803391,3.317021478  H,6.0158701347,2.5492033501,1.9881351691  H,4.7752957057,2.8382821512,-0.1279951711  C,-3.5877182497,1.1791890172,0.2046601237  C,-3.463716274,-0.0173189963,1.0029944755  C,-4.6284820549,-0.5123345292,1.6765211512  H,-4.5328582608,-1.4128046884,2.2762495101  C,-5.8354427357,0.1159459462,1.5802266656  H,-6.6973857525,-0.2846796553,2.1028700402  C,-5.9707792215,1.2917282905,0.7989698595  H,-6.931349153,1.7875491935,0.7255898907  C,-4.8709715856,1.7852030372,0.1436417528  H,-4.9860454397,2.6863179925,-0.4506871483  C,-1.0615079598,0.9394338348,-0.3257391801  C,0.1776345496,1.3205153525,-0.9272474199  H,0.1794967668,2.2143828128,-1.5499990817  C,-1.0664676114,-0.2407739591,0.4883438308  C,-2.3838635671,3.0436806374,-1.4305668869  H,-3.3730383246,3.491549865,-1.5510270123  H,-1.7324611111,3.8241969054,-1.0207066581  H,-2.0047027887,2.8399247923,-2.4382577082  B,-2.3568092089,1.7259947268,-0.5199034718  C,-2.241431788,-0.6864409931,1.1247930085  H,-2.1951783435,-1.584275642,1.7347054853  C,3.0471902988,2.0407799232,-2.4361676973  H,2.4151076149,1.888953507,-3.3178184383  H,2.7913827823,3.0254510761,-2.0286777537  H,4.0834677967,2.1006280454,-2.7884313721  C,2.6539434996,-1.2301305675,0.2021537627  H,2.599582773,-2.1447089232,0.7885525807  B,2.8448869946,0.881009682,-1.3442190806  C,3.1338255087,-1.5472517056,-1.2186222876  O,3.2318548173,-0.4989202861,-1.985103583  O,3.4006269337,-2.6791092623,-1.581396109</p>
<p><i>cis</i>-DBP-CO<sub>2</sub>:CO<sub>2</sub> (THF) ; E=-1276.35874401H</p>	<p>48  C,0.1316849691,-0.5565052714,-1.1830043556  C,1.3045221275,0.0223245178,-0.7971370276</p>



C,1.3469814237,1.1787346792,0.0380350782  
 C,3.5947044018,0.331375795,0.9321629897  
 C,3.464682646,-0.7764454276,0.0783070652  
 C,4.001135658,-2.0132198779,0.3983983326  
 H,3.8894095042,-2.8532253256,-0.2793928256  
 C,4.6798250065,-2.1715685152,1.607098354  
 C,4.8141878188,-1.0934365787,2.4709139689  
 C,4.2746921827,0.1490510782,2.1303644871  
 H,0.1333595899,-1.4334738855,-1.8262452558  
 H,5.0989375573,-3.1356727625,1.8699830256  
 H,5.3417482421,-1.2180315587,3.40986084  
 H,4.3929133914,0.9832889666,2.8162741145  
 C,-3.7107692678,0.9674083062,0.1453519153  
 C,-3.5822388421,-0.1845404955,-0.7141527661  
 C,-4.7737323564,-0.8699280841,-1.1195816142  
 H,-4.674818451,-1.7366142916,-1.7662671958  
 C,-6.0105563787,-0.4643728797,-0.7072595124  
 H,-6.8928425098,-1.0071307249,-1.0294538522  
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 C,-1.1218573089,1.1269301596,0.111206994  
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 H,0.14681147,2.5692962466,1.0994998707  
 C,-1.123500708,-0.0267717079,-0.7395030417  
 C,-2.4787012132,2.9965701806,1.5445954077  
 H,-1.9274398445,3.8297035249,1.0947090429  
 H,-3.4794269327,3.3688393692,1.7755496301  
 H,-1.98646912,2.7991391208,2.5041116654  
 B,-2.4495272257,1.7017699562,0.6030620261  
 C,-2.3277956656,-0.6446135423,-1.1313526903  
 H,-2.280206695,-1.5158848497,-1.778307289  
 C,-2.9228051702,-2.6241471552,1.0812387422  
 O,-2.7178637216,-1.8671959446,1.9275379342  
 O,-3.1349931099,-3.4399696453,0.2886467826  
 C,3.1077288937,3.0495968286,1.0654060258  
 H,2.6303545467,3.8831908477,0.5382947442  
 H,2.6893495264,3.0342152479,2.0781614328  
 H,4.1710074629,3.2971929197,1.1626897754  
 C,2.6826982589,-0.4897340885,-1.1926556266  
 H,2.6424263549,-1.3430539021,-1.8661376589  
 B,2.8744228155,1.6528254151,0.3092430318  
 C,3.39549288,0.6820599186,-1.8771942333  
 O,3.4965339462,1.7435133336,-1.1296977882  
 O,3.8250188998,0.6112511824,-3.0147831352

*cis*-DBP-(CO<sub>2</sub>)<sub>2</sub> (THF) ; E=-1276.39683801H

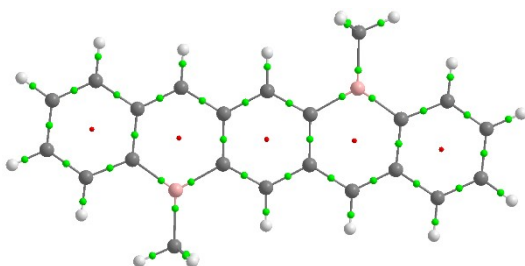
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 H,-4.1526474649,2.2910152435,-2.0341793715  
 C,-5.2471955,2.2367128465,-0.1770668498  
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 H,0.0744403669,1.2841675641,-2.2284280471  
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C,3.6585233955,-0.4702948423,0.4106462088  
C,3.5745804869,0.2320657971,-0.8019330829  
C,4.3940975663,-0.0659205154,-1.8779781366  
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C,5.3201822215,-1.1037310309,-1.7638873708  
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C,4.5899272586,-1.4966601824,0.5025483329  
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H,-0.0557657189,-1.1763900801,2.084115518  
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H,3.6983736098,-0.2864223386,3.4369325569  
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H,2.4875528967,1.882124324,-1.7400240453  
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O,2.897549218,1.639685957,1.5100928257  
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H,-2.1280088634,-3.0973995823,1.7730390063  
H,-2.6819970726,-1.7545337401,2.765872013  
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H,-2.3420643026,0.6222315001,-2.6046853997  
C,-2.4208983989,0.1114979527,-1.6475083965  
B,-2.6440911434,-1.2598080062,0.5695124405  
O,-2.9057783766,-2.0396607008,-0.7643975357  
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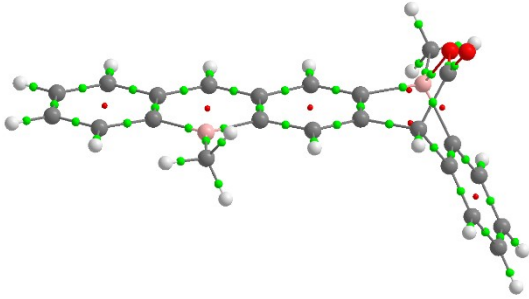
**trans-DBP<sup>(2-)</sup>**

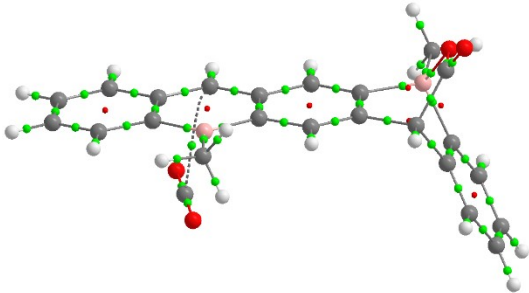
*trans*-DBP (THF) ; E=-899.102188017H



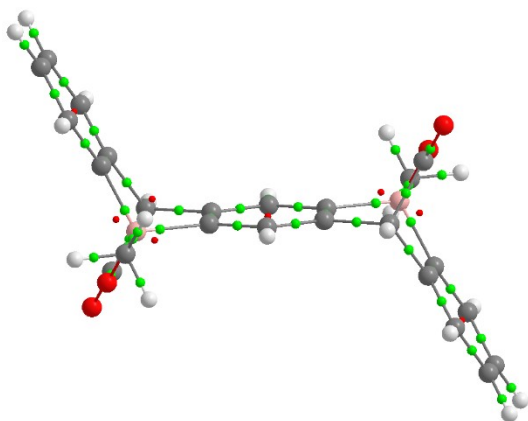
42  
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C,3.8417384553,0.5345177315,0.0087282967  
C,5.1738364415,1.0338481575,0.0099567965  
H,5.3163887302,2.1103163273,0.0075832036  
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C,6.1096397104,-1.181904815,0.0171018747  
C,4.8623095148,-1.7257225677,0.0161403046  
H,0.0415919822,2.4676361263,-0.0028945943  
H,2.3470130705,-2.5832740826,0.0136399755  
H,7.2805794091,0.6563996963,0.0147560512  
H,6.9799931611,-1.8294995812,0.0202875775  
H,4.7427311223,-2.805243366,0.0185657857  
B,2.6123095099,1.4255310164,0.0042738049  
C,2.6656900109,3.0235303857,0.0005346731  
H,3.673197493,3.4450622268,0.0013156371  
H,2.149823891,3.4343466215,-0.87499296



	<p>H,2.1467318384,3.4385180263,0.8722629245  C,-3.8566710632,-0.5338321868,-0.0025514483  C,-3.6903394731,0.9103852956,-0.0057831396  C,-4.8772437305,1.7264085167,-0.0098998998  H,-4.7576656526,2.805929383,-0.0123247656  C,-6.1245727582,1.182590182,-0.0107999589  H,-6.9949270077,1.8301841511,-0.0139394231  C,-6.2992134358,-0.2305300377,-0.0076576995  H,-7.2955133473,-0.6557144156,-0.0084001486  C,-5.1887697169,-1.0331629966,-0.0037117626  H,-5.3313195489,-2.109631598,-0.0013362978  C,-1.2630200426,-0.6985269201,0.0024972865  C,-0.0432656064,-1.3785707898,0.0063587271  H,-0.056523074,-2.4669505032,0.0090008138  C,-1.2270715273,0.7454148368,-0.0009646933  C,-2.433618021,1.4995976427,-0.0049717519  H,-2.3619461784,2.5839600591,-0.0074909313  C,-2.6806196221,-3.0228446591,0.0056454441  H,-2.1648258185,-3.4335844459,0.8812548612  H,-3.6881241398,-3.4443819025,0.0048212252  H,-2.1615848683,-3.4379004882,-0.8660015318  B,-2.627244575,-1.424845411,0.0018192244</p>
<p><i>trans</i>-DBP-CO<sub>2</sub> (THF); E=-1087.75598316H</p> 	<p>45  C,0.0801130998,-0.6517914666,-1.2661174804  C,1.3031545564,-0.1411359026,-0.9351070021  C,1.3474063871,0.9842252622,-0.0555286459  C,3.5372902679,0.2882481447,0.8440654793  C,3.5800911362,-0.8433102499,0.0130195499  C,4.2464524765,-1.9689759011,0.481818464  H,4.2970028851,-2.8624962171,-0.1342148528  C,4.8581663408,-1.9725259241,1.7373522539  C,4.8094055382,-0.8400923165,2.538335167  C,4.1464141058,0.3020690363,2.0887654191  H,0.011722016,-1.5079744084,-1.9360754102  H,5.3740595,-2.8590281303,2.0886101612  H,5.2845409021,-0.8414693773,3.5122558992  H,4.1029351984,1.1892809094,2.7119875786  B,2.7988198123,-0.5854194006,-1.3909416226  C,2.9370737869,-1.7069834805,-2.5306871148  H,3.9835691514,-1.9062605777,-2.789048006  H,2.499371501,-2.6605959631,-2.2146801177  H,2.4280665849,-1.4151076517,-3.4558235435  C,-3.6758275875,0.9935769517,0.1800728907  C,-3.6087049731,-0.1548193182,-0.6923363201  C,-4.8357072146,-0.7738719491,-1.0999988077  H,-4.7835249251,-1.6369951569,-1.757199884  C,-6.0486804233,-0.3064123893,-0.6858359678  H,-6.9585056134,-0.7981955948,-1.012932528  C,-6.1279868384,0.8205337794,0.1713097377  H,-7.0935294429,1.1878907268,0.4979205773  C,-4.9679128086,1.4314523969,0.5757274477  H,-5.0404286266,2.2930144603,1.2322665758  C,-1.0892539073,1.0461655687,0.0982641813  C,0.2034862559,1.5522401174,0.4279428899  H,0.2726405788,2.41515728,1.0871179123  C,-1.1466700724,-0.0944479089,-0.7692909245  C,-2.3327601704,2.9452806775,1.593235825  H,-1.7674675577,3.7677105796,1.1408003408  H,-3.3125974127,3.3475155026,1.8608204426</p>

	<p>H,-1.8201927458,2.7140303396,2.5343147087  B,-2.378589992,1.6675833524,0.6277607732  C,2.7615132327,1.4551093701,0.2577589804  H,2.7825257373,2.339483256,0.8911031633  C,3.4109229305,1.7660237867,-1.0939419985  O,3.8606536437,2.862864034,-1.3732462091  O,3.4298272011,0.7491221271,-1.9107691089  C,-2.3822513422,-0.6607873746,-1.137263665  H,-2.3825001734,-1.5249640001,-1.7957942094</p>
<p><i>trans</i>-DBP-CO<sub>2</sub>:CO<sub>2</sub> (THF) ; E=-1276.35965321H</p> 	<p>48  C,0.0870984869,-0.6153592499,-1.3080113847  C,1.3121751961,-0.1117898027,-0.9715822815  C,1.359000992,1.0158863259,-0.0958203457  C,3.5213107003,0.2950811034,0.842456549  C,3.5589688737,-0.8431029483,0.0199036999  C,4.199376337,-1.9754143393,0.5081890603  H,4.2466630979,-2.8739790231,-0.1006999846  C,4.7911033947,-1.9786120856,1.7735121281  C,4.7495058785,-0.838897498,2.5646773872  C,4.1114383171,0.3098337934,2.0960901987  H,0.0161805452,-1.4734939931,-1.9752887094  H,5.2870862871,-2.8703781868,2.1398078135  H,5.2101349139,-0.8397684311,3.5455573283  H,4.0723943908,1.2028062739,2.711197398  B,2.8080563885,-0.5805590677,-1.4005567769  C,2.9471217889,-1.7118891423,-2.5305677909  H,3.9936835471,-1.9290745258,-2.7728084116  H,2.4908065649,-2.6565363242,-2.213736586  H,2.4547404766,-1.4186743167,-3.4644044119  C,-3.6644179418,1.0057125384,0.1791007956  C,-3.5999699615,-0.1331617843,-0.7043981606  C,-4.8248709172,-0.7747325243,-1.0803917733  H,-4.7743059007,-1.6321182695,-1.7447875175  C,-6.0341947729,-0.3401930209,-0.6187191155  H,-6.9429729106,-0.8505988432,-0.9194258419  C,-6.1102408101,0.7770545314,0.2498091497  H,-7.0722470352,1.1190137585,0.6124660581  C,-4.9505613966,1.4132535493,0.6184274731  H,-5.0209527242,2.2677067673,1.2842898758  C,-1.0773606293,1.0823831101,0.0601734862  C,0.2160886626,1.5884803594,0.3857861687  H,0.2887274576,2.4493904465,1.04705714  C,-1.1379429309,-0.0548954129,-0.8110257001  C,-2.3204130924,2.9669536567,1.5743232528  H,-1.7468204046,3.786976259,1.1281653516  H,-3.3000116563,3.3735899965,1.8359027331  H,-1.8159408852,2.7301058804,2.5185688073  B,-2.3660638733,1.6911338222,0.6073027077  C,2.7742203836,1.4703402994,0.2353398724  H,2.7975268339,2.3573998496,0.8646026063  C,3.4564278004,1.7614087763,-1.1038288726  O,3.9367803152,2.8465560279,-1.3780253444  O,3.4715829722,0.7401684536,-1.9151199664  C,-2.3747203421,-0.6239245155,-1.1720639674  H,-2.3773722162,-1.4846229115,-1.8348036194  C,-2.9659086391,-2.633123208,1.0194152053  O,-2.7077748362,-1.9020737903,1.873984031  O,-3.2321937259,-3.4232063645,0.2173162846</p>

*Trans*-DBP-(CO<sub>2</sub>)<sub>2</sub> (THF) ; E=-1276.39772984H

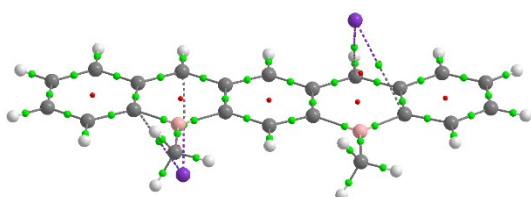


48

C,0.0272251427,1.3640903079,-0.2467775079  
C,1.1090813318,0.7800375961,0.4104676497  
C,1.0644698351,-0.5990360095,0.645052892  
C,3.5264021577,-0.7865125072,0.5246438117  
C,3.6645458744,0.5886973049,0.2782616844  
C,4.7442247232,1.0052363449,-0.4899354862  
H,4.8823739395,2.062047056,-0.70065066  
C,5.66419972,0.0839584991,-0.9970915094  
C,5.5134233397,-1.2694447687,-0.7307969528  
C,4.4369921267,-1.7109351,0.0399283353  
H,0.0210434173,2.4336504423,-0.4471763245  
H,6.5000005753,0.4249317927,-1.597569489  
H,6.2271831809,-1.9843970838,-1.1226662793  
H,4.3117195709,-2.7682885889,0.2487501618  
B,2.4752951831,1.4422717812,0.9924589113  
C,2.5997573168,3.0423233326,0.9801579415  
H,3.5350095126,3.3874819389,1.4356898515  
H,2.5766340724,3.4407477684,-0.0405302487  
H,1.779660934,3.520623003,1.5272477536  
C,-3.6555266066,-0.6061319748,-0.2722050936  
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C,-4.4279656572,1.6934975393,-0.0337996924  
H,-4.3026930228,2.7508561957,-0.2425952854  
C,-5.5043956335,1.2519874779,0.7369158171  
H,-6.218153053,1.9669299528,1.1288074532  
C,-5.6551759158,-0.1014236578,1.0031683654  
H,-6.490975523,-0.442412336,1.6036393542  
C,-4.7352045045,-1.0226894184,0.4959834165  
H,-4.873352927,-2.0795052034,0.706673555  
C,-1.1000602293,-0.7974598412,-0.404398229  
C,-0.0182046744,-1.3815135569,0.2528463938  
H,-0.0120236285,-2.4510734833,0.4532465292  
C,-1.0554500006,0.5816136536,-0.6389853984  
C,-2.5907158359,-3.0597441521,-0.9741302759  
H,-2.5676118878,-3.4581823303,0.0465529384  
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H,-1.7706056399,-3.5380324431,-1.5212093463  
B,-2.4662627616,-1.4596915187,-0.9864084354  
C,2.3008928606,-1.1435860421,1.3501074601  
H,2.2315706796,-2.2069137096,1.5682219089  
C,2.4322996003,-0.3499157545,2.6547484583  
O,2.4507019936,-0.8825755824,3.7495234314  
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H,-2.2225659107,2.1895043259,-1.5621159311  
C,-2.4233597131,0.3325268478,-2.648665731  
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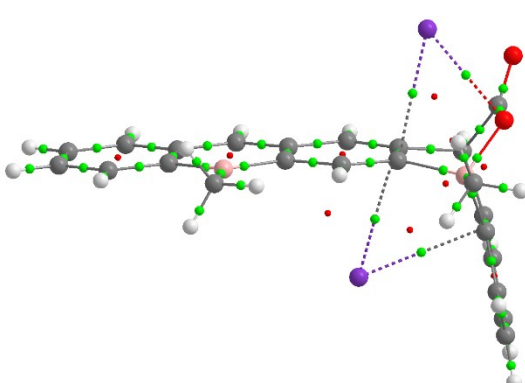
***cis*-DBP<sup>(2-)</sup>:2K<sup>(+)</sup>**

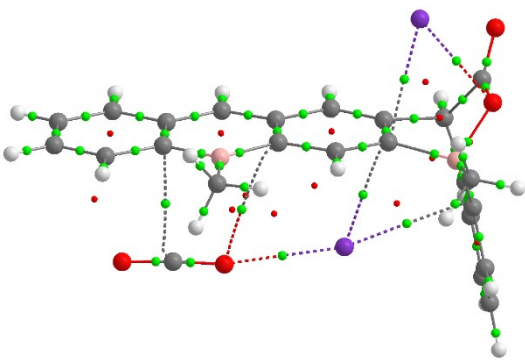
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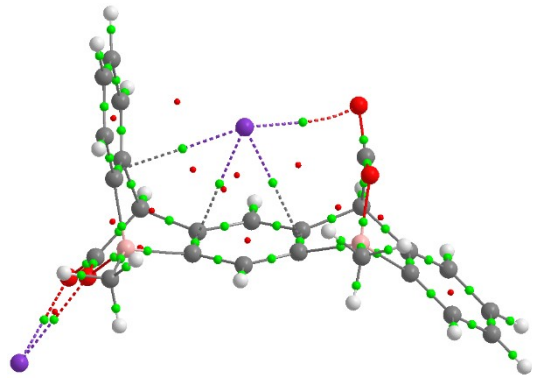


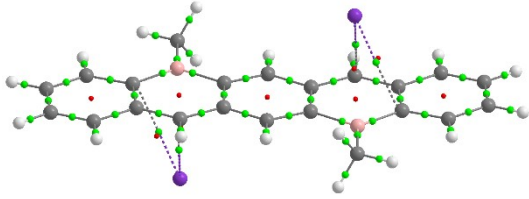
44

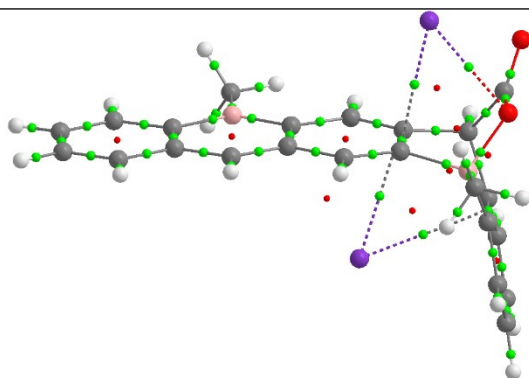
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C,1.2003961024,-0.8982112171,-0.0481212064  
C,3.7956262622,-0.967777985,-0.0230987844  
C,3.7561674697,0.476864815,-0.0411832921  
C,5.002192602,1.1871604262,-0.0050498667  
H,4.9770978687,2.2719972206,-0.0212113425

	<p>C,6.1975415973,0.5325503264,0.0450883585  C,6.2478684288,-0.8837336489,0.064295019  C,5.0730870375,-1.5886606163,0.0289701087  H,0.1537232705,2.3814132368,-0.0028872166  H,7.1205410514,1.1011823926,0.0691153039  H,7.2025869347,-1.3928967525,0.1017667122  H,5.1169782434,-2.6725113532,0.0387194196  C,-3.8639982896,-0.4864087117,0.0213619768  C,-3.6506480892,0.9392275646,0.0340130838  C,-4.8012817093,1.7937583831,-0.0075417025  H,-4.6474818948,2.8680375288,0.002751598  C,-6.0668830829,1.285380254,-0.0547396486  H,-6.9153550435,1.960023569,-0.0826099305  C,-6.2868429334,-0.1143545199,-0.0655151315  H,-7.2959168316,-0.5052755047,-0.0996670448  C,-5.2036634885,-0.9542200584,-0.0268380177  H,-5.3705317497,-2.0272858763,-0.029178727  C,-1.2817868114,-0.7521591429,0.050412455  C,-0.0770416036,-1.4664124775,0.0014341355  H,-0.1361688216,-2.5510554664,0.000189235  C,-1.1834723032,0.7013874914,0.048602583  C,-2.3598462869,1.490764574,0.0447292793  H,-2.2577014409,2.5716693191,0.0492074893  C,-2.8660813915,-3.0107016979,0.1280186253  H,-3.4628885715,-3.2975518586,1.0008259248  H,-3.4269211675,-3.3701209666,-0.7420060691  H,-1.9422149566,-3.5897836309,0.1715458286  B,-2.6608468931,-1.4320863288,0.0838914168  K,-2.3788598125,0.1999703438,-2.5842517317  K,2.4104290403,-0.0904566977,2.5825430877  C,2.3991388753,-3.3407823326,-0.1142680901  H,1.8599711171,-3.738041482,0.7530014786  H,1.8381996341,-3.6828212822,-0.9908730076  H,3.3677299294,-3.8426759093,-0.1433390265  B,2.4815541045,-1.7506908523,-0.0800512319  H,2.5836546135,2.272247157,-0.0592228866  C,2.5466634661,1.1871624476,-0.0510157242</p>
<p><i>cis</i>-DBP-K<sub>2</sub>-CO<sub>2</sub> (THF); E=-2287.50644215H</p> 	<p>47  C,3.6198342431,-3.3520449405,0.6414101471  C,3.5088149192,-2.1189718936,1.289166612  C,3.2615482074,-0.9541736854,0.5688287664  C,3.1453888536,-1.0556411208,-0.8282073003  C,3.2668932222,-2.2709702556,-1.4858171378  C,3.5004831641,-3.4281768079,-0.7410135224  C,2.6909640658,0.2189811725,-1.5153671727  C,1.3217734574,0.5250721459,-0.8986516936  C,1.374517063,0.7198215287,0.5234564971  C,0.1725132076,0.8543575781,1.1785094832  H,0.1869210234,0.9852177116,2.2581646686  C,-1.0996627317,0.775484217,0.5353742835  C,-1.1110407313,0.5931836373,-0.9005548186  C,0.1493335157,0.4817906037,-1.589261023  H,3.801476466,-4.2525390191,1.2157208202  H,3.6006891744,-2.0759488316,2.3699726132  H,3.1626231256,-2.3264089072,-2.5638410031  H,3.5882953955,-4.3838892839,-1.2425114858  H,2.6549473801,0.1412045912,-2.598611039  H,0.1466081773,0.3221793687,-2.663998175  B,2.8875344838,0.5311548999,1.1031982728</p>

	<p>C,3.1572320602,0.8800318062,2.6396831284  H,2.5834407924,0.2275990539,3.3060816239  H,2.8754442427,1.9076611086,2.8994977766  H,4.2119184472,0.7609098725,2.9077751856  C,3.5370683879,1.4082623828,-1.0919175575  O,3.7394489325,1.4968713327,0.1983044495  O,3.8665506611,2.2970975163,-1.8586398927  C,-3.5659223006,0.5435966522,-0.993438972  C,-3.6850126822,0.7142862685,0.4238402187  C,-4.7549447375,0.4273225807,-1.7738633603  C,-4.9933338857,0.7569955756,0.9700778193  C,-5.9929181629,0.4751074483,-1.1965827146  H,-6.8806449296,0.3848710687,-1.81230579  C,-6.1241015111,0.6422207871,0.2011382481  H,-7.108393176,0.6795414476,0.6516993543  H,-5.0995827444,0.8869589457,2.0428349348  H,-4.6606798304,0.2992760934,-2.8474889539  K,2.1146412488,3.6162811484,0.1064353267  C,-2.5433523714,1.050102464,2.8674480476  H,-3.1260745592,1.9460766278,3.1084972264  H,-1.5884390435,1.1462964622,3.3880582303  H,-3.0770609975,0.2158320272,3.3363390904  C,-2.30247576,0.4864405092,-1.6171160086  H,-2.2568794852,0.3524297378,-2.6932755191  B,-2.4267470226,0.8490858209,1.2884951289  K,0.404803745,-2.0650014472,0.2650401865</p>
<p><i>cis</i>-DBP-K<sub>2</sub>-CO<sub>2</sub>:CO<sub>2</sub> (THF); E=-2476.11416168H</p> 	<p>50  C,4.7750858521,-1.6087344399,-0.0776276796  C,4.2322584372,-0.683826188,0.81801112  C,3.5425139125,0.4340176717,0.3585856832  C,3.4253754423,0.6107925007,-1.030688417  C,3.9709328874,-0.2918613857,-1.9314823204  C,4.6463286335,-1.4133285662,-1.4472913873  C,2.5058353226,1.7452046205,-1.4441158025  C,1.143487344,1.3775282817,-0.8462225923  C,1.1677126576,1.2582908807,0.5840023916  C,0.0239093761,0.7904955478,1.1892143015  H,0.0245305509,0.6749617098,2.2708135164  C,-1.1459702025,0.3877726802,0.4782011407  C,-1.1349645635,0.5322102677,-0.9604297435  C,0.049349821,1.0546438217,-1.5899425023  H,5.3008701063,-2.4800554909,0.294016491  H,4.3385784613,-0.8519047317,1.8852004125  H,3.8585840797,-0.1396314039,-2.999349905  H,5.0692928517,-2.1293549186,-2.1408360207  H,2.4638200351,1.9029342587,-2.5184451044  H,0.0707293815,1.1465652219,-2.6723896104  B,2.6618472025,1.5168297745,1.1854371605  C,2.8371621725,1.5887315922,2.772948804  H,2.5683193514,0.6401677537,3.2493762758  H,2.2062009133,2.3553247207,3.2390184155  H,3.8703749228,1.8081805283,3.0608195944  C,2.8644089366,3.0364534712,-0.7275867152  O,3.0630912212,2.9042236434,0.5595755576  O,2.8150351566,4.1309253377,-1.2627538744  C,-3.3958020773,-0.4037577456,-1.1916184005  C,-3.5194004356,-0.6142472066,0.221268227  C,-4.4881372354,-0.7628578076,-2.037734615  C,-4.7329585105,-1.1770378076,0.6951956127</p>

	<p>C,-5.6364755731,-1.2986076586,-1.5276752628  H,-6.4521789875,-1.5611311603,-2.1918935927  C,-5.7696837338,-1.5145659269,-0.1366378888  H,-6.6831639991,-1.9412259737,0.2594565188  H,-4.8410952643,-1.3429573483,1.7628963291  H,-4.3919231826,-0.5997858209,-3.1065464153  K,0.7682969726,4.2351569981,0.8548920425  C,-2.4896601274,-0.4565729979,2.7310739408  H,-3.3717090398,0.0450672079,3.1438250294  H,-1.6306595774,-0.1112139606,3.3097978744  H,-2.6196963055,-1.5201526269,2.9625365533  C,-2.2213845932,0.1440098147,-1.745939842  H,-2.1659251343,0.2801510668,-2.8215050325  B,-2.3720555868,-0.2204168741,1.1569817606  K,1.2708986447,-1.5616288506,-0.3254282954  C,-2.1689616596,-3.285703752,-0.7678820278  O,-1.0916676188,-2.9058185836,-0.5686778547  O,-3.2113612392,-3.724257146,-0.9724418511</p>
<p><i>cis</i>-DBP-K<sub>2</sub>-(CO<sub>2</sub>)<sub>2</sub> (THF) ; E=-2476.14978875H</p> 	<p>50  C,0.17270445,-0.4513574008,-1.552211801  C,1.3181275723,-0.1065685289,-0.8399251459  C,1.3465056477,-0.098728888,0.5615614112  C,3.9415155285,0.0208227138,0.4246054782  C,3.8182842447,0.0062324796,-0.9704979148  C,4.81814105,-0.4981285982,-1.7876261852  H,4.7038562128,-0.4911538184,-2.8662896973  C,5.9712973266,-1.0210860862,-1.2059023055  C,6.1108737259,-1.0253290287,0.1757576728  C,5.1011605996,-0.5027850768,0.9840264297  H,0.1537184279,-0.3966966617,-2.6366577687  H,6.7576445157,-1.4236250165,-1.8329274251  H,7.0099329853,-1.4318856317,0.6240619197  H,5.2286087473,-0.5039349033,2.0623322648  C,-3.1576521132,0.4849203949,0.4604820761  C,-3.060523395,0.4441030958,-0.9405466233  C,-3.418904187,1.5216446323,-1.7342678199  H,-3.325995872,1.4678640147,-2.8133099446  C,-3.8740525104,2.6925909139,-1.1225911202  H,-4.1442718951,3.5477471151,-1.7294505564  C,-3.976619712,2.7586525485,0.2607463982  H,-4.3292793038,3.6688403653,0.7307948265  C,-3.6276262718,1.6548625096,1.0460511351  H,-3.7107523913,1.7240246013,2.1262160606  C,-0.9946618993,-0.7745407672,0.5680722505  C,0.190961056,-0.4820259694,1.2460154448  H,0.1861116501,-0.4553358779,2.3337736269  C,-0.9765080321,-0.7566641952,-0.8327732288  C,-2.7189540213,-1.0502407995,2.7264758407  H,-2.2752865761,-0.2313421708,3.3021584598  H,-3.7783866459,-1.0885896451,3.0017691257  H,-2.2504572631,-1.9723790249,3.0866759631  B,-2.5094662579,-0.8399458369,1.1571212044  C,-2.3617294615,-0.8026133989,-1.4767627826  H,-2.3302332461,-0.8424376616,-2.5622192963  C,-3.0835702354,-2.0117278578,-0.9219875842  O,-3.1767257912,-2.0311982139,0.3820052514  O,-3.5411784502,-2.9134656114,-1.6102415328  C,2.7177034964,0.9860555839,2.7044050939  H,1.8298395646,1.5172491804,3.064930825</p>

	<p>H,2.7869996645,0.0574669842,3.2814845586  H,3.5866834927,1.595362695,2.9739135132  H,2.4527256992,0.5996668964,-2.5747501492  C,2.5196727378,0.5790757573,-1.4899639319  B,2.656556376,0.6894025417,1.1347025266  K,-4.1871717894,-4.460621486,0.446104582  K,-0.5574522537,2.2776035908,-0.1037395065  O,2.4829540386,2.0744687245,0.3641603645  C,2.3158799277,1.9887777603,-0.9234776881  O,1.8759417264,2.9088980866,-1.5987564762</p>
<b><i>trans</i> DBP<sup>(2-)</sup>:2K<sup>(+)</sup></b>	
<p><i>trans</i>-DBP-K<sub>2</sub> (THF) ; E=-2098.85138358H</p> 	<p>44  C,0.0284041387,1.3835068119,0.0158224917  C,1.2453550769,0.7004470701,-0.0395347834  C,1.2080132456,-0.7467729847,-0.0573356185  C,2.4148747786,-1.5005216733,-0.0700926807  C,3.6753609382,-0.9050946281,-0.0616998444  C,3.8361941159,0.5368436237,-0.0317404298  C,5.1714125031,1.040616892,0.0149952387  H,5.3116668528,2.1161601823,0.0349965784  C,6.2751106614,0.2360962192,0.0329449705  C,6.1032646175,-1.1770717297,0.0016787239  C,4.8590435802,-1.7234507886,-0.0427986533  H,0.0424599015,2.4707505113,0.0261209074  H,2.3464035053,-2.5838624879,-0.09079409  H,7.2716492444,0.65831926,0.0660148478  H,6.9751117542,-1.8215614236,0.0114543941  H,4.7376280516,-2.8016763183,-0.0687913532  B,2.6092545977,1.433485801,-0.0663404783  C,2.6611843688,3.0254242548,-0.0773486942  H,3.6684023967,3.4454832638,-0.0903790069  H,2.1396854961,3.4245893322,-0.954731447  H,2.1464880621,3.4552243301,0.789596771  C,-3.8535496354,-0.5361592781,0.0315762806  C,-3.6927161787,0.9057783233,0.0615340343  C,-4.8763969703,1.7241362227,0.0426383938  H,-4.7549793721,2.8023615258,0.0686299124  C,-6.12061923,1.1777589007,-0.001830909  H,-6.9924658227,1.8222493552,-0.0116013115  C,-6.2924661568,-0.2354084945,-0.033094228  H,-7.2890051308,-0.6576312845,-0.0661569817  C,-5.1887688326,-1.0399306938,-0.015150804  H,-5.329026267,-2.1154735341,-0.0351485488  C,-1.2627111296,-0.6997645076,0.0393726922  C,-0.0457587983,-1.3828242137,-0.015985905  H,-0.0598156857,-2.4700679547,-0.0262839483  C,-1.2253691691,0.7474551608,0.057174683  C,-2.4322286479,1.5012047018,0.069928477  H,-2.363756768,2.5845455399,0.0906253616  C,-2.6785464834,-3.0247409521,0.0772011116  H,-3.6857680013,-3.4447934037,0.0901719549  H,-2.1637938443,-3.4545647548,-0.7896979074  H,-2.1571116662,-3.4238918315,0.9546291494  B,-2.6266096952,-1.4328026192,0.066179022  K,-2.466070338,0.2350891455,-2.5760140304  K,2.4487924556,-0.2344179916,2.5758600574</p>
<p><i>trans</i>-DBP-K<sub>2</sub>-CO<sub>2</sub> (THF); E=-2287.50714851H</p>	<p>47  C,-3.6637732658,-3.3695767064,-0.3885101112</p>

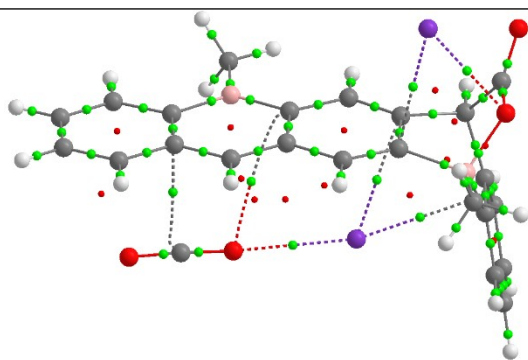


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 C,-3.2808830409,-0.9822707571,-0.5779170299  
 C,-3.1778568046,-0.9280511164,0.8228223201  
 C,-3.3212259796,-2.0618323653,1.6097189211  
 C,-3.5600640454,-3.2920725193,0.9951781519  
 C,-2.7064201952,0.4080605519,1.3631459076  
 C,-1.3339769524,0.6382895007,0.7177600787  
 C,-1.3745785568,0.6529137375,-0.7183226018  
 C,-0.1920618272,0.7137488134,-1.4003206442  
 H,-0.193734092,0.7193855241,-2.4886810642  
 C,1.087151381,0.7105108665,-0.7309662057  
 C,1.1109012555,0.6781017055,0.7162680163  
 C,-0.1430939831,0.6652865363,1.3930054144  
 H,-3.8491160441,-4.3265736043,-0.861155214  
 H,-3.6123332873,-2.2938886056,-2.2475090102  
 H,-3.228320832,-1.998174985,2.6883732255  
 H,-3.6642020071,-4.1852011737,1.5986809128  
 H,-2.6702515652,0.4515338863,2.4484814791  
 H,-0.1510113218,0.6334731047,2.4788382056  
 B,-2.894575744,0.4305350763,-1.2751573375  
 C,-3.1580914103,0.6077952199,-2.8409761175  
 H,-2.5886087275,-0.1187984385,-3.4297273647  
 H,-2.8680366115,1.5993220414,-3.2081920097  
 H,-4.2133253606,0.46812486,-3.0966215304  
 C,-3.5356534129,1.5517757901,0.8110124  
 O,-3.7140026295,1.5107617647,-0.4868493742  
 O,-3.8653831383,2.5216595648,1.4732333752  
 C,3.6907981737,0.623789652,0.5442159267  
 C,3.5410583593,0.6614845711,-0.8796699359  
 C,5.0098252783,0.5818729619,1.0633517131  
 C,4.7127668884,0.6538340171,-1.693713215  
 C,6.1238547365,0.5756010608,0.2618958762  
 H,7.1174731531,0.5438393744,0.6919329095  
 C,5.9627512141,0.6121872044,-1.1419584141  
 H,6.8370184052,0.6082814202,-1.7830400416  
 H,4.5956915538,0.682857181,-2.7723258692  
 H,5.1385323252,0.5546503926,2.1411631391  
 K,-1.9932637405,3.5942028961,-0.47293952  
 K,-0.432902962,-2.0855947413,-0.0332383086  
 B,2.4516630957,0.6353509988,1.4459621575  
 C,2.5971291052,0.6022740167,3.0341432423  
 H,3.1308962233,-0.2949613271,3.366822571  
 H,3.1905982703,1.4500927673,3.3935251535  
 H,1.6508969275,0.6278971008,3.5785368411  
 C,2.2639739132,0.702984683,-1.4780868545  
 H,2.1962421519,0.7276122925,-2.5612779473

*trans*-DBP-K<sub>2</sub>-CO<sub>2</sub>:CO<sub>2</sub> (THF); E=-2476.114914H

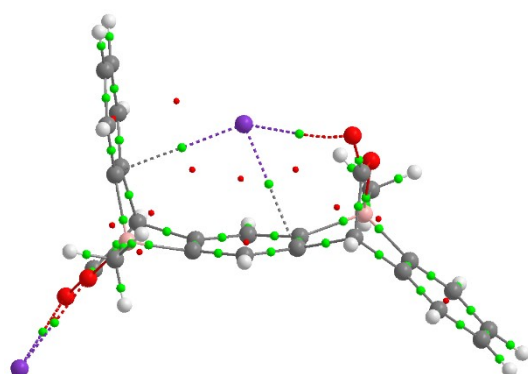
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 C,4.7080787009,-1.6057359895,0.230071414  
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 C,3.4746182696,0.5647258166,-0.966128462  
 C,4.057585129,-0.4107260078,-1.7621028697  
 C,4.6731834885,-1.5067936545,-1.1555939137  
 C,2.6021697418,1.6775179278,-1.5142633499  
 C,1.1972354618,1.3901482396,-0.9690743933  
 C,1.1390709766,1.3535952825,0.4649708476  
 C,-0.0308373069,0.9675828043,1.0569926449  
 H,-0.1004138419,0.924312746,2.1423145325  
 C,-1.1803441121,0.5469698423,0.2934224264





C,-1.0994417539,0.5719396868,-1.1503401033  
 C,0.1177402884,1.0295444004,-1.7312577458  
 H,5.1869209062,-2.4582400393,0.6965695154  
 H,4.1629220476,-0.7004671631,2.1007130989  
 H,4.0180726567,-0.3346002476,-2.8432213879  
 H,5.1229758282,-2.2794404055,-1.7667134576  
 H,2.6222901178,1.7535853975,-2.5982987295  
 H,0.2063352253,1.0498734847,-2.8136943214  
 B,2.602372906,1.6461579925,1.1301999181  
 C,2.68631837,1.8353150628,2.7146459745  
 H,2.3693021262,0.931650026,3.2454429459  
 H,2.0452917128,2.6477647042,3.0772262629  
 H,3.7051200832,2.0592645212,3.0466603196  
 C,2.9453971638,3.0115977779,-0.8793721393  
 O,3.0442862762,2.9767748844,0.4273268254  
 O,2.9592954676,4.0644230377,-1.4952519477  
 C,-3.4976697779,-0.3975426935,-1.1732907607  
 C,-3.4687182352,-0.3532290056,0.2592478777  
 C,-4.6844263663,-0.8722300379,-1.789601604  
 C,-4.6232528305,-0.7780697812,0.9828729357  
 C,-5.7822961619,-1.276103503,-1.0735770502  
 H,-6.6734030382,-1.6315018357,-1.5765469294  
 C,-5.7426729006,-1.2227016079,0.3386156308  
 H,-6.6068837221,-1.5388267431,0.9119136102  
 H,-4.5983358878,-0.7409771561,2.067397527  
 H,-4.7209259068,-0.911955272,-2.8741350664  
 K,0.7152188085,4.3316616981,0.3385225933  
 K,1.2376486701,-1.5146330938,-0.3471494277  
 C,-2.2458643919,-3.1897568465,-0.3967163859  
 O,-1.1541535852,-2.8222988953,-0.5310912199  
 O,-3.3045963112,-3.6162454576,-0.2630023364  
 B,-2.2823928747,0.0739294332,-1.9784210296  
 C,-2.2921209157,0.0234985386,-3.5730246738  
 H,-2.4332151407,-1.0013977149,-3.9352232124  
 H,-3.1285152616,0.5996634118,-3.9834119548  
 H,-1.385148283,0.4033242252,-4.0478663234  
 C,-2.324641624,0.0948894892,0.9511778685  
 H,-2.3412451014,0.1015507078,2.0367163308

*trans*-DBP-K<sub>2</sub>-(CO<sub>2</sub>)<sub>2</sub> (THF); E=-2476.15066939H



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 C,-0.2313758679,0.3401267351,-1.6175112341  
 C,-1.4642320299,0.2538166387,-0.9709969431  
 C,-1.485845409,0.3888282104,0.4240828385  
 C,-3.9602391506,0.7867939912,0.4176166352  
 C,-4.0302922518,0.6645489955,-0.9759335943  
 C,-5.0345848856,1.3557647891,-1.6433430999  
 H,-5.1174061019,1.2798604035,-2.7233542196  
 C,-5.944967151,2.1464003993,-0.9419351971  
 C,-5.8616819995,2.2466576772,0.4405686166  
 C,-4.8647760118,1.5589092216,1.1297691407  
 H,-0.1676705326,0.2063427207,-2.6944970657  
 H,-6.7228394118,2.681301317,-1.4742069236  
 H,-6.5709913292,2.8582574264,0.984963102  
 H,-4.7952821603,1.6327172816,2.2097453827  
 C,2.7953714311,-1.0618906281,0.6120292284  
 C,2.7506607512,-1.1117404955,-0.791394203  
 C,2.9189478862,-2.29602158,-1.4904469634  
 H,2.8712756492,-2.30923988,-2.5736876846  
 C,3.1213833787,-3.4810361681,-0.7782306617  
 H,3.2405810293,-4.4163591607,-1.3107604721

C,3.1670561947,-3.4580992179,0.609532823  
H,3.3234237501,-4.379393296,1.1577079717  
C,3.0132780423,-2.2506451823,1.2989504309  
H,3.0486371717,-2.2503479956,2.3839372839  
C,0.9147005962,0.5879551178,0.5302131634  
C,-0.3237647288,0.5762254029,1.1701088427  
H,-0.3802954637,0.6290888356,2.2544611632  
C,0.9331317499,0.4688760824,-0.8656202612  
C,2.5864111161,0.6996342189,2.7427968486  
H,1.9732143989,0.0276000145,3.3521601156  
H,3.6231040695,0.5562832732,3.0656924135  
H,2.2941659403,1.7196150213,3.0146232735  
B,2.393489996,0.4119027199,1.1836733315  
C,2.3223934194,0.1993964183,-1.4447636077  
H,2.3337392079,0.1605737609,-2.5306453457  
C,3.2464201291,1.2880457591,-0.9434618646  
O,3.3010574404,1.3909738408,0.3592821393  
O,3.891316816,2.029835989,-1.671379225  
K,4.7678968569,3.5771591903,0.294522294  
K,-0.0792761649,-2.3625478604,0.0720956365  
B,-2.8820265381,-0.3118805435,-1.5514515949  
C,-2.9384108041,-0.7347779546,-3.0921677615  
H,-3.9040081616,-1.1748627213,-3.3621055711  
H,-2.7875448767,0.1305263452,-3.7469182824  
H,-2.1680742773,-1.4688350825,-3.3532226406  
C,-2.8272649688,0.0178785467,1.05736004  
H,-2.8083414112,0.0864620521,2.1420642924  
O,-3.0242496796,-1.622870179,-0.6587466051  
C,-2.890689851,-1.4506164354,0.6240490161  
O,-2.6695121224,-2.3716395354,1.3984031082

Table S2. Comparison of the relative energies ( $\text{kJ mol}^{-1}$ ) of eight minima calculated at the M06-2X/def2TZVP, PBE0-D3/def2TZVP and DLPNO-CCSD(T)/def2TZVP computational levels. The differences with respect to M06-2x calculations are shown in parenthesis

System	Erel(M06-2X)	Erel(PBE0-D3)	Erel(DLPNO-CCSD(T))
BBZN-CO <sub>2</sub> adduct	-23.3	-22.8 (-0.5)	-25.2 (1.9)
BBZN-K-CO <sub>2</sub> adduct	8.8	6.3 (2.5)	3.5 (5.2)
BA-CO <sub>2</sub> adduct	-113.6	-115.8 (2.2)	-118.0 (4.4)
BA-K-CO <sub>2</sub> adduct	-97.9	-103.1 (5.2)	-101.3 (3.4)
<i>trans</i> -DBP-CO <sub>2</sub> adduct	-157.1	-157.3 (0.2)	- <sup>a</sup>
<i>trans</i> -DBP-K-CO <sub>2</sub> adduct	-152.7	-151.8 (0.9)	- <sup>a</sup>
<i>trans</i> -DBP-(CO <sub>2</sub> ) <sub>2</sub> adduct	-284.6	-287.7 (3.1)	- <sup>a</sup>
<i>trans</i> -DBP-K-(CO <sub>2</sub> ) <sub>2</sub> adduct	-257.7	-257.7 (0.0)	- <sup>a</sup>

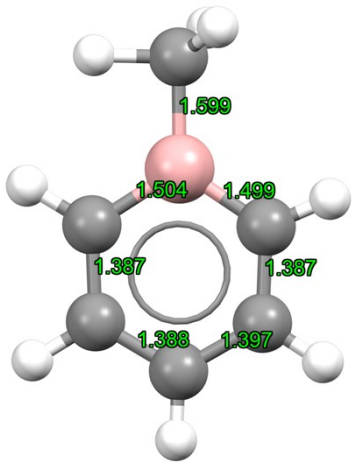
<sup>a</sup> The DLPNO-CCSD(T)/def2TZVP for these systems was not affordable.

Table S3. Comparison of the relative energies ( $\text{kJ mol}^{-1}$ ) computed with the SMD implicit solvent model and with two THF molecules interacting with the potassium cation and the SMD model. Energy differences are shown in parenthesis.

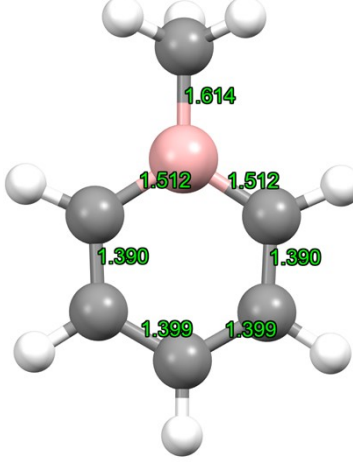
System	Relative energy SMD (in $\text{kJ/mol}$ )	Relative energy two THF molecules + SMD (in $\text{kJ/mol}$ )
TS 1 BBZN-K	+48.1	+50.0 (-1.9)
Inter 1 BBZN-K	+30.1	+31.2 (-1.1)
Adduct BBZN-K	-1.5	0.1 (-1.6)
TS 1 BA-K	+7.5	+7.2 (+0.3)
Inter 1 BA-K	-52.2	-47.4 (-4.8)
Adduct BA-K	-118.2	-114.9 (-3.3)

Table S4. Bond distances ( $\text{\AA}$ ) of the 1methyl-boratabenzene.

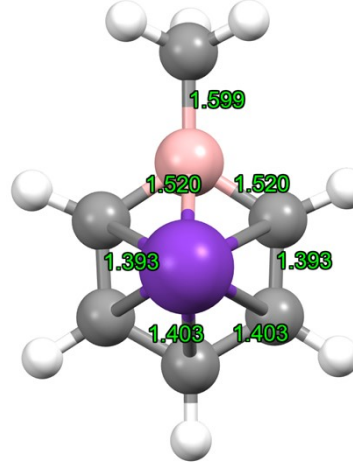
	B-C <sub>ortho</sub>	C <sub>ortho</sub> -C <sub>meta</sub>	C <sub>meta</sub> -C <sub>para</sub>	B-CH <sub>3</sub>
Exp. (YIYBEN)	1.504/1.499	1.387/1.387	1.388/1.397	1.599
Calc. (anion)	1.512	1.390	1.399	1.614
Calc. (K <sup>+</sup> )	1.520	1.393	1.403	1.599



Exp. (CSD Refcode YIYBEN)



Calc.



Calc. with K<sup>+</sup>

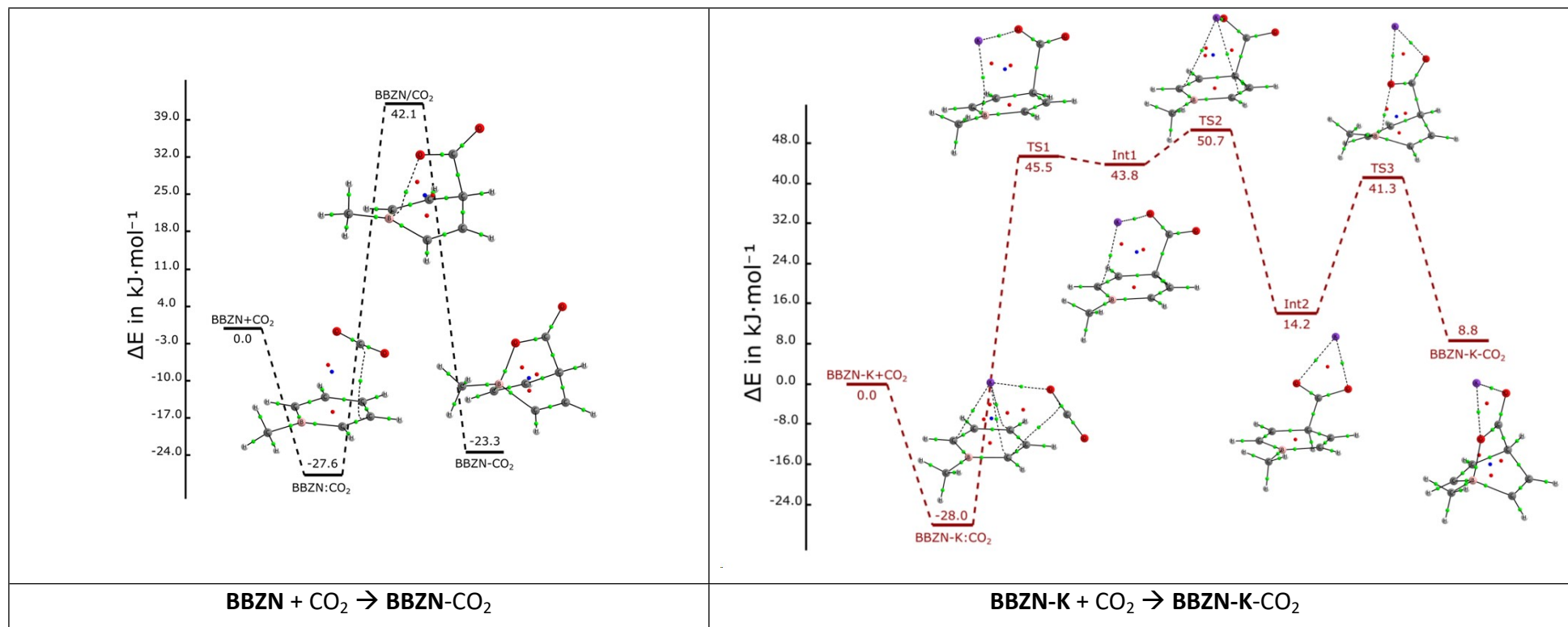
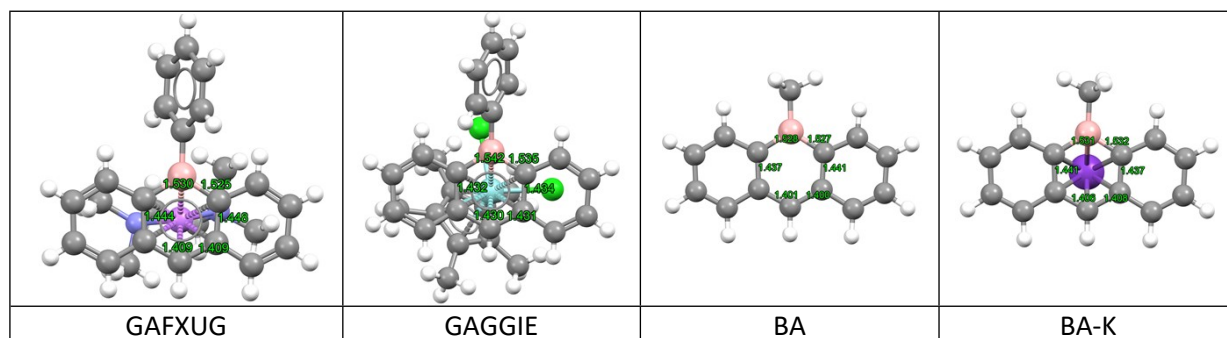


Fig. S1. Energy profiles for the reactions  $\text{BBZN} + \text{CO}_2 \rightarrow \text{BBZN-CO}_2$  (left) and  $\text{BBZN-K} + \text{CO}_2 \rightarrow \text{BBZN-K-CO}_2$  (right) with the corresponding molecular graphs of the stationary points. Green, red and blue small spheres indicate the location of the bond, ring and cage critical points.

Fig. S2. X-ray structures of the 9-borataanthracenes refcodes GAFXUG and GAGGIE and the calculated 9-methyl-9-borataanthracene anion and its potassium salt. The bond distances (Å) of the central ring are indicated.



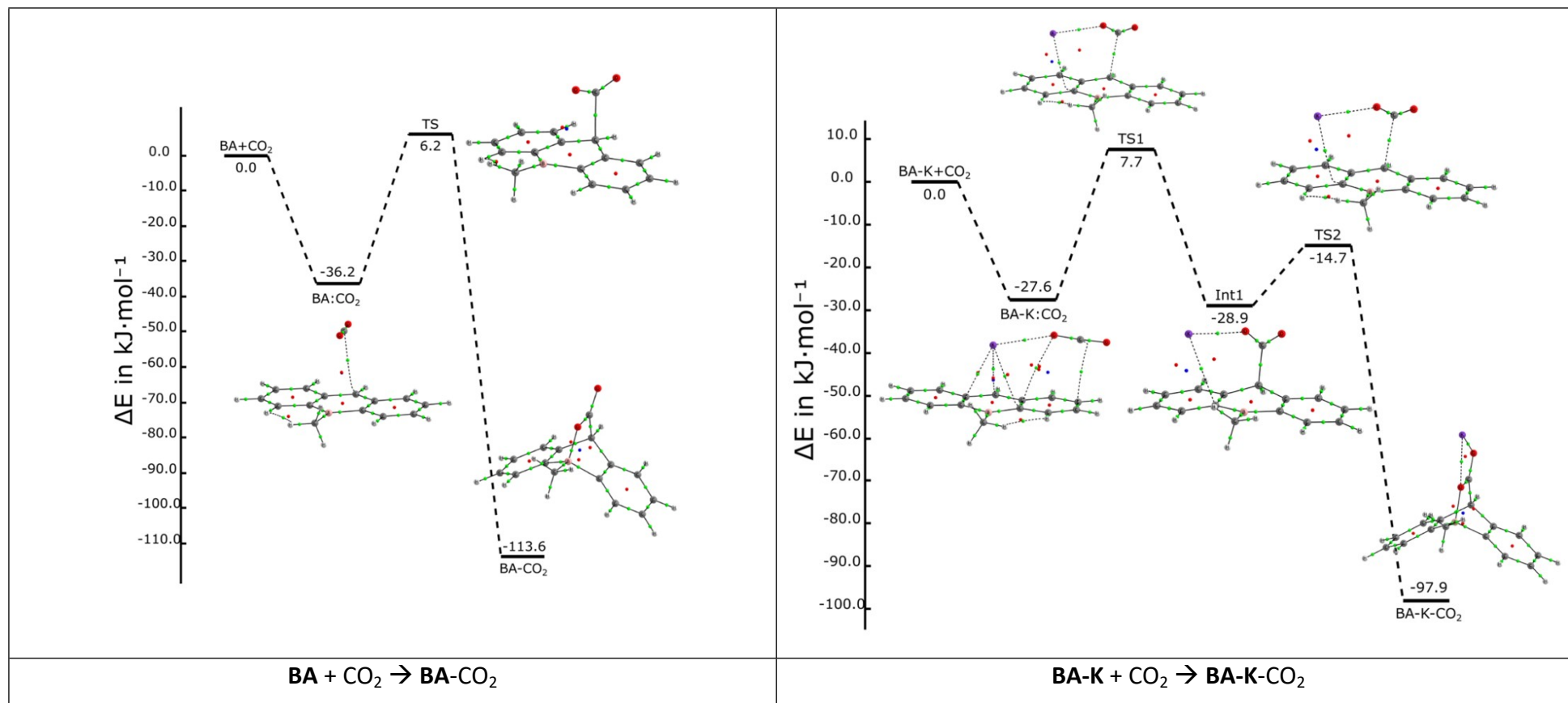


Fig. S3. Energy profiles of reactions  $\text{BA} + \text{CO}_2 \rightarrow \text{BA-CO}_2$  (left) and  $\text{BA-K} + \text{CO}_2 \rightarrow \text{BA-K-CO}_2$  (right) with the molecular graphs of the stationary points.

Figure S4: Optimized geometry of BA:CO<sub>2</sub>, BA-K:CO<sub>2</sub>(1) and BA-K:CO<sub>2</sub>(2) complexes (M06-2X/def2TZVP)

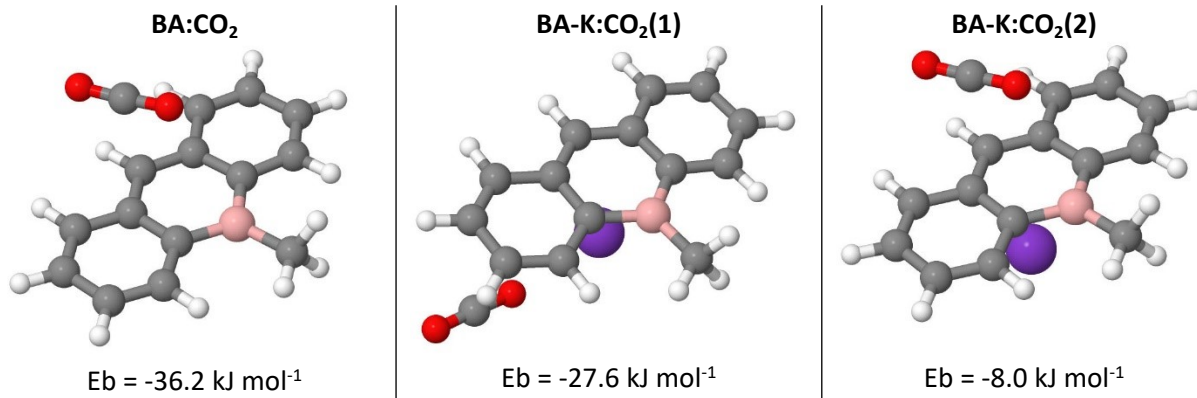


Fig. S5: Superposition of the crystal (green) and optimized (blue) structures of the diboratapentacene derivatives. The corresponding CSD refcode used is indicated.

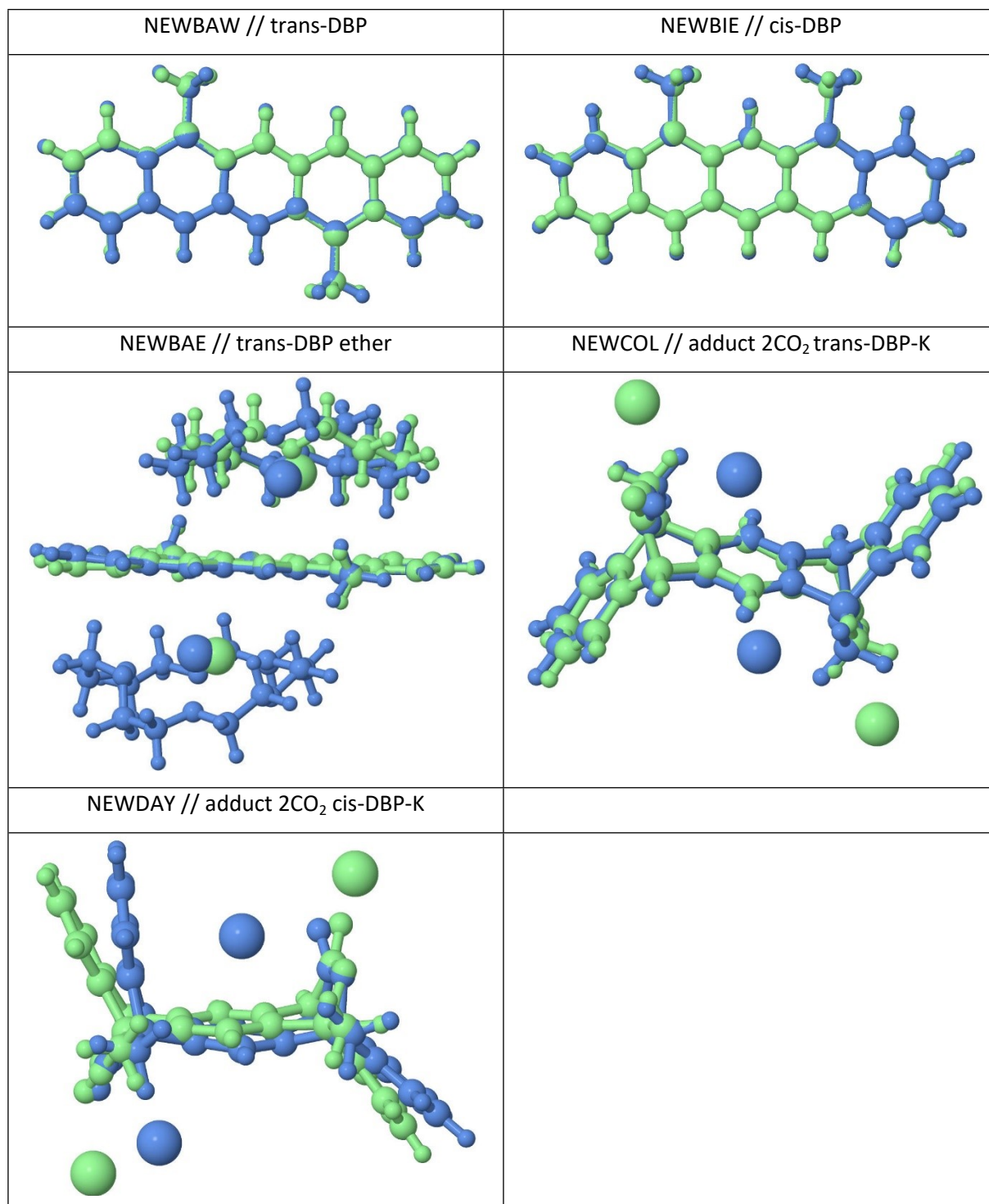




Fig. S6: Scan of the two CO<sub>2</sub> angle capture by the trans-DBP calculated at M06-2X/def2SVP level.

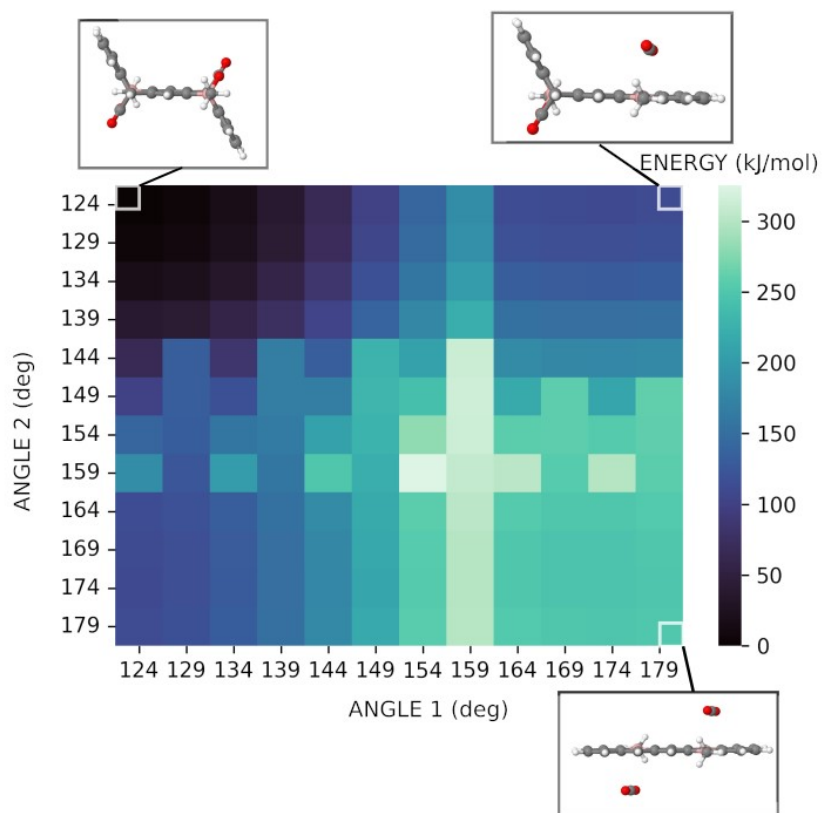


Fig. S7. Energetic profile (kJ mol<sup>-1</sup>) of the formation of the syn adducts with two CO<sub>2</sub> molecules

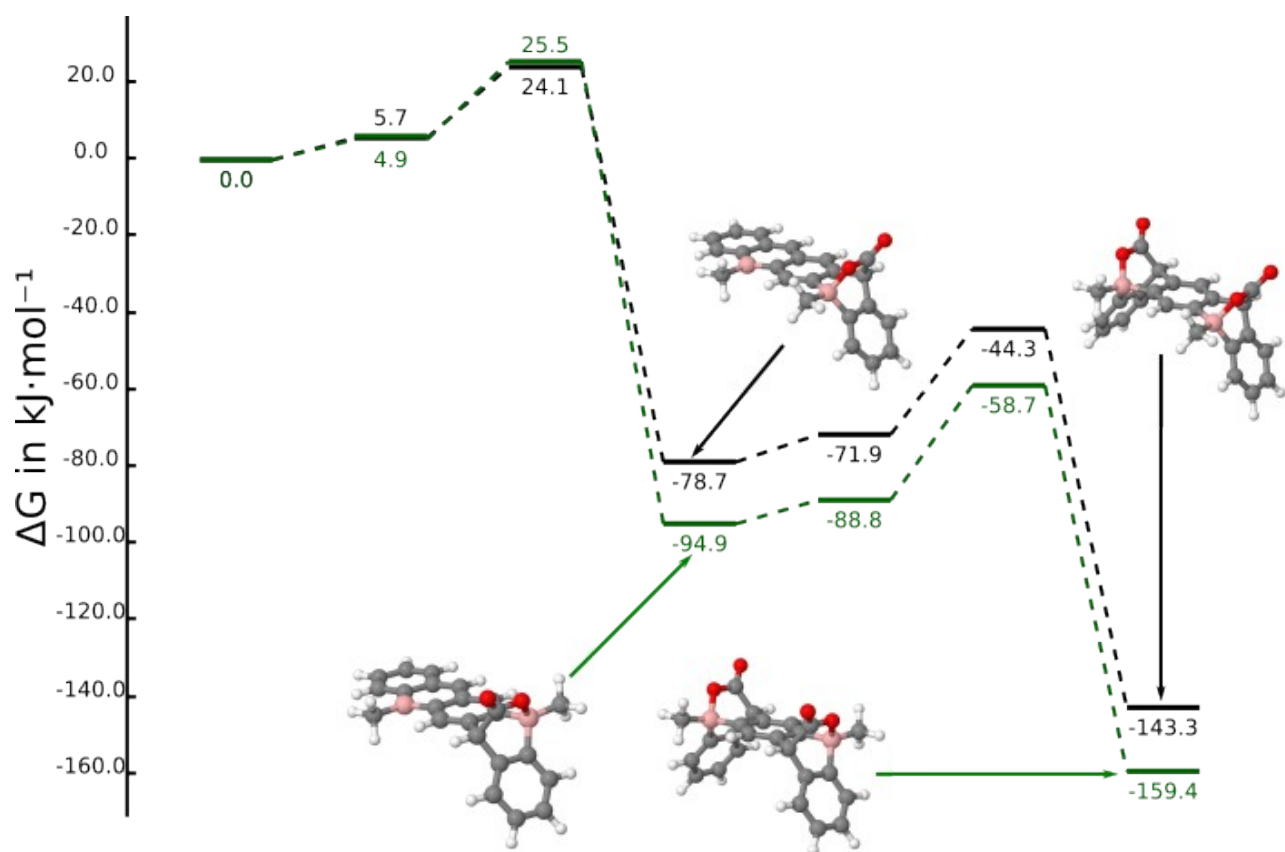


Fig. S8. Reaction profile of *cis*- (green) and *trans*-DBP-K (black) with two CO<sub>2</sub> molecules.

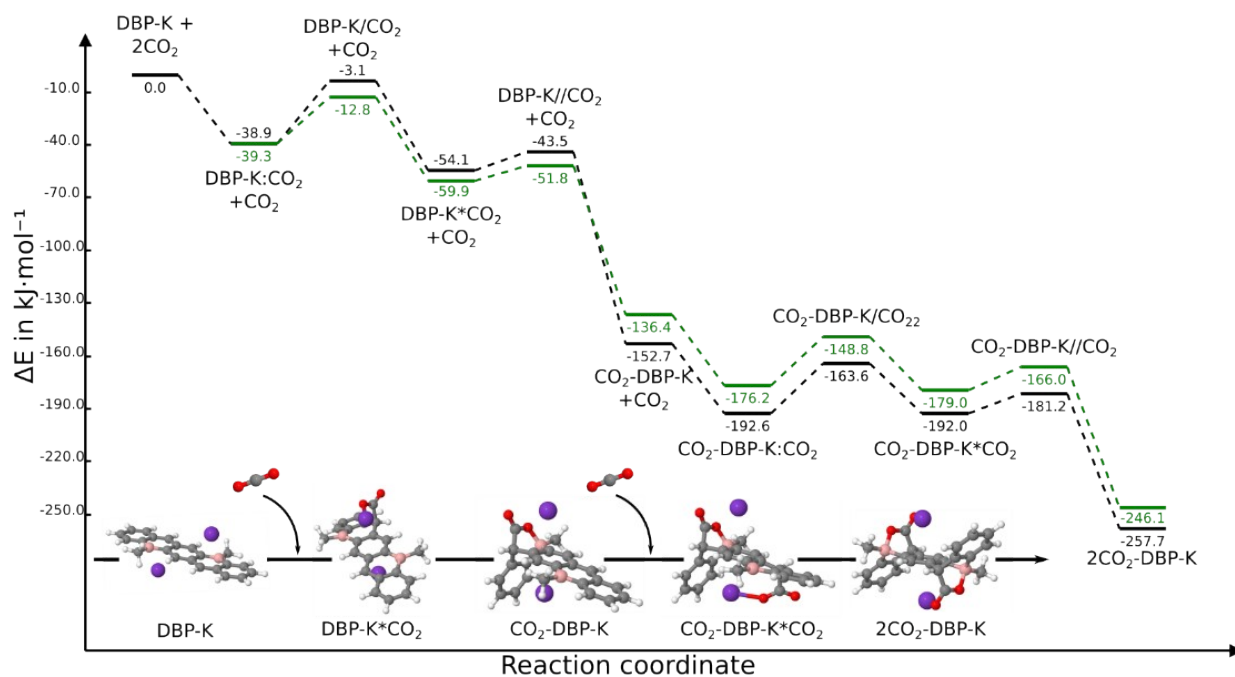


Fig. S9. Syn products of the addition of two CO<sub>2</sub> molecules to the cis and trans-DBP-K molecules.

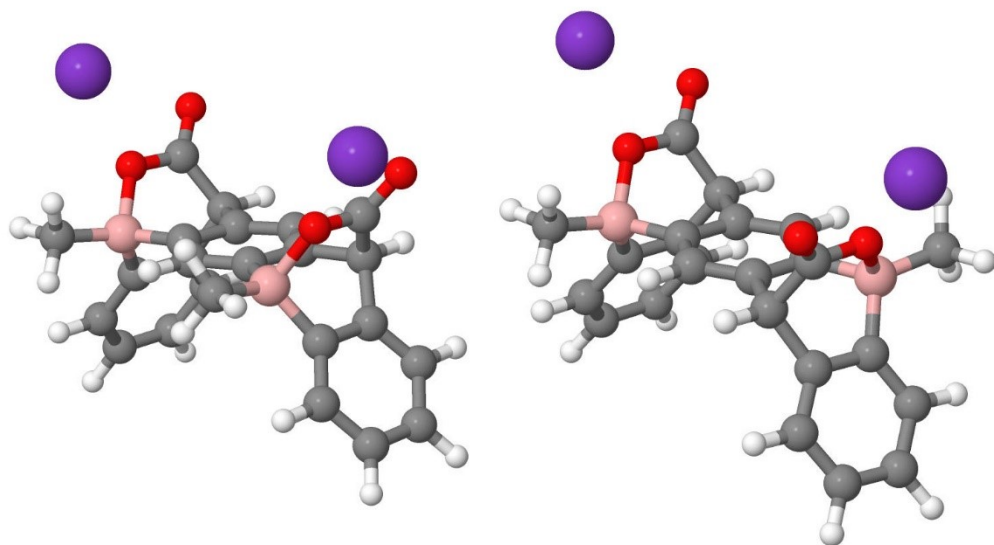
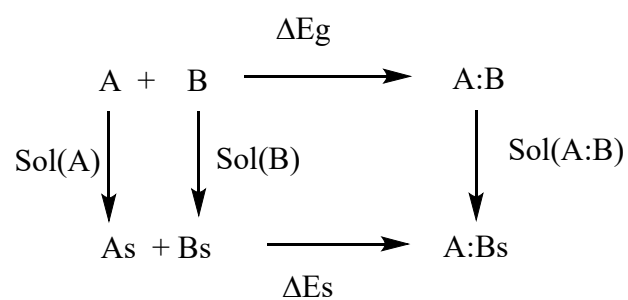


Fig. S10. Solvation thermodynamic cycle and the energetic relations derived from them.



$$\Delta E_g = \text{Sol(A)} + \text{Sol(B)} + \Delta E_s - \text{Sol(A:B)}$$

$$\Delta E_g - \Delta E_s = \text{Sol(A)} + \text{Sol(B)} - \text{Sol(A:B)}$$

g = gas, s = solvated, sol = solvation energy

Fig. S11. MEP of the trans-diboratapentacene in the presence of two potassium cation atoms and two 18-crown-6-ether molecules and the analogous systems with the adduct of one CO<sub>2</sub> molecule. The geometry and wavefunction of these systems corresponds to M06-2X/def2svp calculations.

