78

p-I p-4C6H4F-H2P

N 2.040524000 0.000000000 0.002510000

N 0.000000000 2.104496000 -0.029426000

N -2.040524000 0.000000000 0.002510000

N 0.000000000 -2.104496000 -0.029426000

C 2.862352000 1.087289000 -0.044472000

C 4.257395000 0.675627000 -0.144569000

C 2.862352000 -1.087289000 -0.044472000

C 4.257395000 -0.675627000 -0.144569000

C 1.130597000 -2.884156000 0.016145000

C 0.683351000 -4.241828000 0.103160000

C -1.130597000 -2.884156000 0.016145000

C -0.683351000 -4.241828000 0.103160000

C -2.862352000 -1.087289000 -0.044472000

C -4.257395000 -0.675627000 -0.144569000

C -2.862352000 1.087289000 -0.044472000

C -4.257395000 0.675627000 -0.144569000

C -1.130597000 2.884156000 0.016145000

C -0.683351000 4.241828000 0.103160000

C 1.130597000 2.884156000 0.016145000

C 0.683351000 4.241828000 0.103160000

C 2.457703000 2.435551000 -0.011265000

C 2.457703000 -2.435551000 -0.011265000

C -2.457703000 -2.435551000 -0.011265000

C -2.457703000 2.435551000 -0.011265000

C 3.520839000 3.491697000 -0.001326000

C 3.520839000 -3.491697000 -0.001326000

C -3.520839000 -3.491697000 -0.001326000

C -3.520839000 3.491697000 -0.001326000

H -1.333503000 -5.096776000 0.169045000

H 1.333503000 -5.096776000 0.169045000

H 5.106300000 -1.333896000 -0.221128000

H 5.106300000 1.333896000 -0.221128000

H 1.333503000 5.096776000 0.169045000

H -1.333503000 5.096776000 0.169045000

H -5.106300000 1.333896000 -0.221128000

H -5.106300000 -1.333896000 -0.221128000

C 3.766170000 4.272741000 -1.136015000

C 4.290667000 3.719103000 1.144825000

C 4.753596000 5.254464000 -1.135375000

C 5.280112000 4.698323000 1.165344000

H 3.184515000 4.104620000 -2.033509000

H 4.954239000 5.857198000 -2.010893000

H 5.876097000 4.883301000 2.048892000

H 4.110394000 3.126194000 2.032415000

C 4.290667000 -3.719103000 1.144825000

C 3.766170000 -4.272741000 -1.136015000

C 5.280112000 -4.698323000 1.165344000

C 4.753596000 -5.254464000 -1.135375000

H 4.110394000 -3.126194000 2.032415000

H 5.876097000 -4.883301000 2.048892000

H 4.954239000 -5.857198000 -2.010893000

H 3.184515000 -4.104620000 -2.033509000

C -3.766170000 -4.272741000 -1.136015000

C -4.290667000 -3.719103000 1.144825000

C -4.753596000 -5.254464000 -1.135375000

C -5.280112000 -4.698323000 1.165344000

H -3.184515000 -4.104620000 -2.033509000

H -4.954239000 -5.857198000 -2.010893000

H -5.876097000 -4.883301000 2.048892000

H -4.110394000 -3.126194000 2.032415000

C -4.290667000 3.719103000 1.144825000

C -3.766170000 4.272741000 -1.136015000

C -5.280112000 4.698323000 1.165344000

C -4.753596000 5.254464000 -1.135375000

H -4.110394000 3.126194000 2.032415000

H -5.876097000 4.883301000 2.048892000

H -4.954239000 5.857198000 -2.010893000

H -3.184515000 4.104620000 -2.033509000

C -5.492020000 5.447880000 0.020161000

C 5.492020000 5.447880000 0.020161000

C 5.492020000 -5.447880000 0.020161000

C -5.492020000 -5.447880000 0.020161000

H 0.000000000 -1.093279000 -0.051124000

H 0.000000000 1.093279000 -0.051124000

F 6.454077000 -6.402111000 0.030586000

F -6.454077000 -6.402111000 0.030586000

F -6.454077000 6.402111000 0.030586000

F 6.454077000 6.402111000 0.030586000

78

p-II p-4C6H4F-H2P

N 0.000000000 0.000000000 2.040514000

N 2.102854000 0.059546000 0.000000000

N 0.000000000 0.000000000 -2.040514000

N -2.102854000 -0.059546000 0.000000000

C 1.087205000 0.003302000 2.863710000

C 0.675586000 0.005218000 4.262444000

C -1.087205000 -0.003302000 2.863710000

C -0.675586000 -0.005218000 4.262444000

C -2.883258000 -0.021670000 1.130398000

C -4.242623000 0.036666000 0.683293000

C -2.883258000 -0.021670000 -1.130398000

C -4.242623000 0.036666000 -0.683293000

C -1.087205000 -0.003302000 -2.863710000

C -0.675586000 -0.005218000 -4.262444000

C 1.087205000 0.003302000 -2.863710000

C 0.675586000 0.005218000 -4.262444000

C 2.883258000 0.021670000 -1.130398000

C 4.242623000 -0.036666000 -0.683293000

C 2.883258000 0.021670000 1.130398000

C 4.242623000 -0.036666000 0.683293000

C 2.434922000 0.009811000 2.457445000

C -2.434922000 -0.009811000 2.457445000

C -2.434922000 -0.009811000 -2.457445000

C 2.434922000 0.009811000 -2.457445000

C 3.493761000 -0.009119000 3.519017000

C -3.493761000 0.009119000 3.519017000

C -3.493761000 0.009119000 -3.519017000

C 3.493761000 -0.009119000 -3.519017000

H -5.098176000 0.087810000 -1.334076000

H -5.098176000 0.087810000 1.334076000

H -1.334124000 -0.015406000 5.114538000

H 1.334124000 0.015406000 5.114538000

H 5.098176000 -0.087810000 1.334076000

H 5.098176000 -0.087810000 -1.334076000

H 1.334124000 0.015406000 -5.114538000

H -1.334124000 -0.015406000 -5.114538000

C 3.788423000 -1.186933000 4.214121000

C 4.210310000 1.150118000 3.834562000

C 4.770903000 -1.214229000 5.200363000

C 5.194974000 1.142651000 4.819231000

H 3.245367000 -2.093406000 3.978771000

H 5.007172000 -2.121467000 5.739966000

H 5.749277000 2.036075000 5.073437000

H 3.990378000 2.071044000 3.309492000

C -3.788423000 1.186933000 4.214121000

C -4.210310000 -1.150118000 3.834562000

C -4.770903000 1.214229000 5.200363000

C -5.194974000 -1.142651000 4.819231000

H -3.245367000 2.093406000 3.978771000

H -5.007172000 2.121467000 5.739966000

H -5.749277000 -2.036075000 5.073437000

H -3.990378000 -2.071044000 3.309492000

C -4.210310000 -1.150118000 -3.834562000

C -3.788423000 1.186933000 -4.214121000

C -5.194974000 -1.142651000 -4.819231000

C -4.770903000 1.214229000 -5.200363000

H -3.990378000 -2.071044000 -3.309492000

H -5.749277000 -2.036075000 -5.073437000

H -5.007172000 2.121467000 -5.739966000

H -3.245367000 2.093406000 -3.978771000

C 4.210310000 1.150118000 -3.834562000

C 3.788423000 -1.186933000 -4.214121000

C 5.194974000 1.142651000 -4.819231000

C 4.770903000 -1.214229000 -5.200363000

H 3.990378000 2.071044000 -3.309492000

H 5.749277000 2.036075000 -5.073437000

H 5.007172000 -2.121467000 -5.739966000

H 3.245367000 -2.093406000 -3.978771000

C 5.455697000 -0.044167000 -5.483539000

C 5.455697000 -0.044167000 5.483539000

C -5.455697000 0.044167000 5.483539000

C -5.455697000 0.044167000 -5.483539000

H -1.091649000 -0.086235000 0.000000000

H 1.091649000 0.086235000 0.000000000

F -6.412903000 0.061257000 6.442649000

F -6.412903000 0.061257000 -6.442649000

F 6.412903000 -0.061257000 -6.442649000

F 6.412903000 -0.061257000 6.442649000

78

p-III p-4C6H4F-H2P

N -0.032893000 2.040004000 0.000000000

N 0.000000000 0.000000000 2.103396000

N 0.032893000 -2.040004000 0.000000000

N 0.000000000 0.000000000 -2.103396000

C 0.001597000 2.862614000 1.087169000

C 0.065482000 4.259923000 0.675593000

C 0.001597000 2.862614000 -1.087169000

C 0.065482000 4.259923000 -0.675593000

C 0.000816000 1.130466000 -2.884420000

C -0.002995000 0.683322000 -4.245069000

C -0.000816000 -1.130466000 -2.884420000

C 0.002995000 -0.683322000 -4.245069000

C -0.001597000 -2.862614000 -1.087169000

C -0.065482000 -4.259923000 -0.675593000

C -0.001597000 -2.862614000 1.087169000

C -0.065482000 -4.259923000 0.675593000

C -0.000816000 -1.130466000 2.884420000

C 0.002995000 -0.683322000 4.245069000

C 0.000816000 1.130466000 2.884420000

C -0.002995000 0.683322000 4.245069000

C 0.003370000 2.457173000 2.435193000

C 0.003370000 2.457173000 -2.435193000

C -0.003370000 -2.457173000 -2.435193000

C -0.003370000 -2.457173000 2.435193000

C 0.014472000 3.521052000 3.491944000

C 0.014472000 3.521052000 -3.491944000

C -0.014472000 -3.521052000 -3.491944000

C -0.014472000 -3.521052000 3.491944000

H 0.009515000 -1.333985000 -5.102193000

H -0.009515000 1.333985000 -5.102193000

H 0.118925000 5.110211000 -1.334442000

H 0.118925000 5.110211000 1.334442000

H -0.009515000 1.333985000 5.102193000

H 0.009515000 -1.333985000 5.102193000

H -0.118925000 -5.110211000 1.334442000

H -0.118925000 -5.110211000 -1.334442000

C -1.149402000 4.234237000 3.798154000

C 1.187025000 3.822710000 4.192657000

C -1.150510000 5.224313000 4.777205000

C 1.205722000 4.810825000 5.173702000

H -2.065531000 4.010458000 3.266512000

H -2.046806000 5.778092000 5.022274000

H 2.109541000 5.054316000 5.715831000

H 2.097747000 3.284199000 3.962954000

C 1.187025000 3.822710000 -4.192657000

C -1.149402000 4.234237000 -3.798154000

C 1.205722000 4.810825000 -5.173702000

C -1.150510000 5.224313000 -4.777205000

H 2.097747000 3.284199000 -3.962954000

H 2.109541000 5.054316000 -5.715831000

H -2.046806000 5.778092000 -5.022274000

H -2.065531000 4.010458000 -3.266512000

C -1.187025000 -3.822710000 -4.192657000

C 1.149402000 -4.234237000 -3.798154000

C -1.205722000 -4.810825000 -5.173702000

C 1.150510000 -5.224313000 -4.777205000

H -2.097747000 -3.284199000 -3.962954000

H -2.109541000 -5.054316000 -5.715831000

H 2.046806000 -5.778092000 -5.022274000

H 2.065531000 -4.010458000 -3.266512000

C 1.149402000 -4.234237000 3.798154000

C -1.187025000 -3.822710000 4.192657000

C 1.150510000 -5.224313000 4.777205000

C -1.205722000 -4.810825000 5.173702000

H 2.065531000 -4.010458000 3.266512000

H 2.046806000 -5.778092000 5.022274000

H -2.109541000 -5.054316000 5.715831000

H -2.097747000 -3.284199000 3.962954000

C -0.031767000 -5.492906000 5.446647000

C 0.031767000 5.492906000 5.446647000

C 0.031767000 5.492906000 -5.446647000

C -0.031767000 -5.492906000 -5.446647000

H 0.000000000 0.000000000 -1.091941000

H 0.000000000 0.000000000 1.091941000

F 0.040232000 6.455561000 -6.400413000

F -0.040232000 -6.455561000 -6.400413000

F -0.040232000 -6.455561000 6.400413000

F 0.040232000 6.455561000 6.400413000

78

p-IV p-4C6H4F-H2P

N 2.038909000 0.000000000 0.000000000

N 0.000000000 0.000000000 2.102434000

N -2.038909000 0.000000000 0.000000000

N 0.000000000 0.000000000 -2.102434000

C 2.862275000 0.003372000 1.087026000

C 4.261207000 -0.000187000 0.675628000

C 2.862275000 -0.003372000 -1.087026000

C 4.261207000 0.000187000 -0.675628000

C 1.130254000 0.000400000 -2.883527000

C 0.683353000 -0.002107000 -4.244419000

C -1.130254000 -0.000400000 -2.883527000

C -0.683353000 0.002107000 -4.244419000

C -2.862275000 0.003372000 -1.087026000

C -4.261207000 -0.000187000 -0.675628000

C -2.862275000 -0.003372000 1.087026000

C -4.261207000 0.000187000 0.675628000

C -1.130254000 0.000400000 2.883527000

C -0.683353000 -0.002107000 4.244419000

C 1.130254000 -0.000400000 2.883527000

C 0.683353000 0.002107000 4.244419000

C 2.456506000 0.002715000 2.434468000

C 2.456506000 -0.002715000 -2.434468000

C -2.456506000 0.002715000 -2.434468000

C -2.456506000 -0.002715000 2.434468000

C 3.520208000 0.006211000 3.492833000

C 3.520208000 -0.006211000 -3.492833000

C -3.520208000 0.006211000 -3.492833000

C -3.520208000 -0.006211000 3.492833000

H -1.334824000 0.006164000 -5.101093000

H 1.334824000 -0.006164000 -5.101093000

H 5.112730000 0.002954000 -1.335195000

H 5.112730000 -0.002954000 1.335195000

H 1.334824000 0.006164000 5.101093000

H -1.334824000 -0.006164000 5.101093000

H -5.112730000 0.002954000 1.335195000

H -5.112730000 -0.002954000 -1.335195000

C 4.151576000 1.196987000 3.866273000

C 3.900757000 -1.180624000 4.127225000

C 5.140071000 1.210402000 4.847068000

C 4.887771000 -1.187075000 5.109742000

H 3.866359000 2.123958000 3.385120000

H 5.632586000 2.126859000 5.143065000

H 5.191205000 -2.100916000 5.602594000

H 3.423870000 -2.111026000 3.845857000

C 4.151576000 -1.196987000 -3.866273000

C 3.900757000 1.180624000 -4.127225000

C 5.140071000 -1.210402000 -4.847068000

C 4.887771000 1.187075000 -5.109742000

H 3.866359000 -2.123958000 -3.385120000

H 5.632586000 -2.126859000 -5.143065000

H 5.191205000 2.100916000 -5.602594000

H 3.423870000 2.111026000 -3.845857000

C -4.151576000 1.196987000 -3.866273000

C -3.900757000 -1.180624000 -4.127225000

C -5.140071000 1.210402000 -4.847068000

C -4.887771000 -1.187075000 -5.109742000

H -3.866359000 2.123958000 -3.385120000

H -5.632586000 2.126859000 -5.143065000

H -5.191205000 -2.100916000 -5.602594000

H -3.423870000 -2.111026000 -3.845857000

C -4.151576000 -1.196987000 3.866273000

C -3.900757000 1.180624000 4.127225000

C -5.140071000 -1.210402000 4.847068000

C -4.887771000 1.187075000 5.109742000

H -3.866359000 -2.123958000 3.385120000

H -5.632586000 -2.126859000 5.143065000

H -5.191205000 2.100916000 5.602594000

H -3.423870000 2.111026000 3.845857000

C -5.488548000 -0.013358000 5.450137000

C 5.488548000 0.013358000 5.450137000

C 5.488548000 -0.013358000 -5.450137000

C -5.488548000 0.013358000 -5.450137000

H 0.000000000 0.000000000 -1.090989000

H 0.000000000 0.000000000 1.090989000

F 6.449840000 -0.016844000 -6.405409000

F -6.449840000 0.016844000 -6.405409000

F -6.449840000 -0.016844000 6.405409000

F 6.449840000 0.016844000 6.405409000

78

p-V p-4C6H4F-H2P

N -2.038205000 0.000000000 0.000000000

N 0.000000000 2.101989000 0.000000000

N 2.038205000 0.000000000 0.000000000

N 0.000000000 -2.101989000 0.000000000

C -2.861653000 1.086858000 0.000000000

C -4.260733000 0.675662000 0.000000000

C -2.861653000 -1.086858000 0.000000000

C -4.260733000 -0.675662000 0.000000000

C -1.130093000 -2.883121000 0.000000000

C -0.683394000 -4.244187000 0.000000000

C 1.130093000 -2.883121000 0.000000000

C 0.683394000 -4.244187000 0.000000000

C 2.861653000 -1.086858000 0.000000000

C 4.260733000 -0.675662000 0.000000000

C 2.861653000 1.086858000 0.000000000

C 4.260733000 0.675662000 0.000000000

C 1.130093000 2.883121000 0.000000000

C 0.683394000 4.244187000 0.000000000

C -1.130093000 2.883121000 0.000000000

C -0.683394000 4.244187000 0.000000000

C -2.455914000 2.433970000 0.000000000

C -2.455914000 -2.433970000 0.000000000

C 2.455914000 -2.433970000 0.000000000

C 2.455914000 2.433970000 0.000000000

C -3.520208000 3.492621000 0.000000000

C -3.520208000 -3.492621000 0.000000000

C 3.520208000 -3.492621000 0.000000000

C 3.520208000 3.492621000 0.000000000

H 1.335529000 -5.100489000 0.000000000

H -1.335529000 -5.100489000 0.000000000

H -5.111813000 -1.335983000 0.000000000

H -5.111813000 1.335983000 0.000000000

H -1.335529000 5.100489000 0.000000000

H 1.335529000 5.100489000 0.000000000

H 5.111813000 1.335983000 0.000000000

H 5.111813000 -1.335983000 0.000000000

C -4.025958000 3.996002000 1.202536000

C -4.025958000 3.996002000 -1.202536000

C -5.014175000 4.977348000 1.212555000

C -5.014175000 4.977348000 -1.212555000

H -3.644581000 3.614655000 2.141346000

H -5.412369000 5.371695000 2.137763000

H -5.412369000 5.371695000 -2.137763000

H -3.644581000 3.614655000 -2.141346000

C -4.025958000 -3.996002000 -1.202536000

C -4.025958000 -3.996002000 1.202536000

C -5.014175000 -4.977348000 -1.212555000

C -5.014175000 -4.977348000 1.212555000

H -3.644581000 -3.614655000 -2.141346000

H -5.412369000 -5.371695000 -2.137763000

H -5.412369000 -5.371695000 2.137763000

H -3.644581000 -3.614655000 2.141346000

C 4.025958000 -3.996002000 1.202536000

C 4.025958000 -3.996002000 -1.202536000

C 5.014175000 -4.977348000 1.212555000

C 5.014175000 -4.977348000 -1.212555000

H 3.644581000 -3.614655000 2.141346000

H 5.412369000 -5.371695000 2.137763000

H 5.412369000 -5.371695000 -2.137763000

H 3.644581000 -3.614655000 -2.141346000

C 4.025958000 3.996002000 -1.202536000

C 4.025958000 3.996002000 1.202536000

C 5.014175000 4.977348000 -1.212555000

C 5.014175000 4.977348000 1.212555000

H 3.644581000 3.614655000 -2.141346000

H 5.412369000 5.371695000 -2.137763000

H 5.412369000 5.371695000 2.137763000

H 3.644581000 3.614655000 2.141346000

C 5.488915000 5.448798000 0.000000000

C -5.488915000 5.448798000 0.000000000

C -5.488915000 -5.448798000 0.000000000

C 5.488915000 -5.448798000 0.000000000

H 0.000000000 -1.090558000 0.000000000

H 0.000000000 1.090558000 0.000000000

F -6.450612000 -6.403729000 0.000000000

F 6.450612000 -6.403729000 0.000000000

F 6.450612000 6.403729000 0.000000000

F -6.450612000 6.403729000 0.000000000

78

p-VI p-4C6H4F-H2P

N 0.000000000 2.092134000 0.000000000

N 0.000000000 0.000000000 2.117395000

N 0.000000000 -2.092134000 0.000000000

N 0.000000000 0.000000000 -2.117395000

C 0.000000000 2.915138000 1.123946000

C 0.000000000 4.280639000 0.662999000

C 0.000000000 2.915138000 -1.123946000

C 0.000000000 4.280639000 -0.662999000

C 0.000000000 1.169164000 -2.903945000

C 0.000000000 0.670166000 -4.227896000

C 0.000000000 -1.169164000 -2.903945000

C 0.000000000 -0.670166000 -4.227896000

C 0.000000000 -2.915138000 -1.123946000

C 0.000000000 -4.280639000 -0.662999000

C 0.000000000 -2.915138000 1.123946000

C 0.000000000 -4.280639000 0.662999000

C 0.000000000 -1.169164000 2.903945000

C 0.000000000 -0.670166000 4.227896000

C 0.000000000 1.169164000 2.903945000

C 0.000000000 0.670166000 4.227896000

C 0.000000000 2.554139000 2.520936000

C 0.000000000 2.554139000 -2.520936000

C 0.000000000 -2.554139000 -2.520936000

C 0.000000000 -2.554139000 2.520936000

C 0.000000000 3.672633000 3.656163000

C 0.000000000 3.672633000 -3.656163000

C 0.000000000 -3.672633000 -3.656163000

C 0.000000000 -3.672633000 3.656163000

H 0.000000000 -1.160219000 -5.159609000

H 0.000000000 1.160219000 -5.159609000

H 0.000000000 5.213537000 -1.154597000

H 0.000000000 5.213537000 1.154597000

H 0.000000000 1.160219000 5.159609000

H 0.000000000 -1.160219000 5.159609000

H 0.000000000 -5.213537000 1.154597000

H 0.000000000 -5.213537000 -1.154597000

C 0.000000000 3.436532000 5.058769000

C 0.000000000 5.076969000 3.435304000

C 0.000000000 4.397876000 6.064962000

C 0.000000000 6.073208000 4.406323000

H 0.000000000 2.473677000 5.487536000

H 0.000000000 4.085433000 7.100660000

H 0.000000000 7.111904000 4.103999000

H 0.000000000 5.509777000 2.474715000

C 0.000000000 3.436532000 -5.058769000

C 0.000000000 5.076969000 -3.435304000

C 0.000000000 4.397876000 -6.064962000

C 0.000000000 6.073208000 -4.406323000

H 0.000000000 2.473677000 -5.487536000

H 0.000000000 4.085433000 -7.100660000

H 0.000000000 7.111904000 -4.103999000

H 0.000000000 5.509777000 -2.474715000

C 0.000000000 -5.076969000 -3.435304000

C 0.000000000 -3.436532000 -5.058769000

C 0.000000000 -6.073208000 -4.406323000

C 0.000000000 -4.397876000 -6.064962000

H 0.000000000 -5.509777000 -2.474715000

H 0.000000000 -7.111904000 -4.103999000

H 0.000000000 -4.085433000 -7.100660000

H 0.000000000 -2.473677000 -5.487536000

C 0.000000000 -3.436532000 5.058769000

C 0.000000000 -5.076969000 3.435304000

C 0.000000000 -4.397876000 6.064962000

C 0.000000000 -6.073208000 4.406323000

H 0.000000000 -2.473677000 5.487536000

H 0.000000000 -4.085433000 7.100660000

H 0.000000000 -7.111904000 4.103999000

H 0.000000000 -5.509777000 2.474715000

C 0.000000000 -5.732054000 5.737256000

C 0.000000000 5.732054000 5.737256000

C 0.000000000 5.732054000 -5.737256000

C 0.000000000 -5.732054000 -5.737256000

H 0.000000000 0.000000000 -1.105823000

H 0.000000000 0.000000000 1.105823000

F 0.000000000 6.680768000 6.696092000

F 0.000000000 -6.680768000 6.696092000

F 0.000000000 -6.680768000 -6.696092000

F 0.000000000 6.680768000 -6.696092000

78

m-I(I) m-4C6H4F-H2P

N 0.000198000 2.040240000 0.003487000

N -2.104301000 0.001046000 -0.027958000

N -0.000198000 -2.040240000 0.003487000

N 2.104301000 -0.001046000 -0.027958000

C -1.086438000 2.863107000 -0.035515000

C -0.674555000 4.259079000 -0.121931000

C 1.087395000 2.862226000 -0.037001000

C 0.676467000 4.258547000 -0.122956000

C 2.884521000 1.129195000 0.009921000

C 4.243120000 0.682284000 0.084290000

C 2.884479000 -1.131231000 0.011384000

C 4.243120000 -0.684192000 0.085413000

C 1.086438000 -2.863107000 -0.035515000

C 0.674555000 -4.259079000 -0.121931000

C -1.087395000 -2.862226000 -0.037001000

C -0.676467000 -4.258547000 -0.122956000

C -2.884521000 -1.129195000 0.009921000

C -4.243120000 -0.682284000 0.084290000

C -2.884479000 1.131231000 0.011384000

C -4.243120000 0.684192000 0.085413000

C -2.434037000 2.457394000 -0.008884000

C 2.434697000 2.455440000 -0.011117000

C 2.434037000 -2.457394000 -0.008884000

C -2.434697000 -2.455440000 -0.011117000

C -3.489900000 3.521755000 0.003790000

C 3.492198000 3.518361000 -0.004852000

C 3.489900000 -3.521755000 0.003790000

C -3.492198000 -3.518361000 -0.004852000

H 5.098866000 -1.334214000 0.141732000

H 5.098588000 1.332827000 0.138938000

H 1.335066000 5.108087000 -0.189130000

H -1.332917000 5.108902000 -0.186637000

H -5.098866000 1.334214000 0.141732000

H -5.098588000 -1.332827000 0.138938000

H -1.335066000 -5.108087000 -0.189130000

H 1.332917000 -5.108902000 -0.186637000

C -4.251723000 3.773527000 -1.141914000

C -3.730407000 4.275613000 1.157887000

C -5.220862000 4.762509000 -1.103015000

C -4.713525000 5.261673000 1.168029000

H -4.090335000 3.217369000 -2.055562000

H -4.891817000 5.834716000 2.069112000

H -3.147198000 4.082602000 2.048694000

C 4.253589000 3.778893000 -1.149552000

C 3.730867000 4.265361000 1.153328000

C 5.232199000 4.769655000 -1.139557000

C 4.712713000 5.242150000 1.134548000

H 4.069146000 3.209103000 -2.050919000

H 5.809284000 4.965471000 -2.034413000

H 3.165959000 4.090076000 2.058925000

C 4.251723000 -3.773527000 -1.141914000

C 3.730407000 -4.275613000 1.157887000

C 5.220862000 -4.762509000 -1.103015000

C 4.713525000 -5.261673000 1.168029000

H 4.090335000 -3.217369000 -2.055562000

H 4.891817000 -5.834716000 2.069112000

H 3.147198000 -4.082602000 2.048694000

C -4.253589000 -3.778893000 -1.149552000

C -3.730867000 -4.265361000 1.153328000

C -5.232199000 -4.769655000 -1.139557000

C -4.712713000 -5.242150000 1.134548000

H -4.069146000 -3.209103000 -2.050919000

H -5.809284000 -4.965471000 -2.034413000

H -3.165959000 -4.090076000 2.058925000

C -5.474278000 -5.516278000 0.010682000

C -5.473959000 5.517811000 0.029793000

C 5.474278000 5.516278000 0.010682000

C 5.473959000 -5.517811000 0.029793000

H 1.092980000 -0.001271000 -0.044731000

H -1.092980000 0.001271000 -0.044731000

H 6.241948000 -6.279062000 0.011851000

H 6.228747000 6.290407000 0.044319000

H -6.241948000 6.279062000 0.011851000

H -6.228747000 -6.290407000 0.044319000

F 5.948504000 -4.999813000 -2.222195000

F 4.936525000 5.956702000 2.264695000

F -5.948504000 4.999813000 -2.222195000

F -4.936525000 -5.956702000 2.264695000

78

m-I(II) m-4C6H4F-H2P

N 0.000000000 2.038706000 0.000000000

N 0.000000000 0.000000000 -2.102665000

N 0.000000000 -2.038706000 0.000000000

N 0.000000000 0.000000000 2.102665000

C -0.005097000 2.862257000 -1.086659000

C -0.001304000 4.261283000 -0.675550000

C 0.005097000 2.862257000 1.086659000

C 0.001304000 4.261283000 0.675550000

C -0.000219000 1.129911000 2.883893000

C 0.002063000 0.683266000 4.244893000

C 0.000219000 -1.129911000 2.883893000

C -0.002063000 -0.683266000 4.244893000

C -0.005097000 -2.862257000 1.086659000

C -0.001304000 -4.261283000 0.675550000

C 0.005097000 -2.862257000 -1.086659000

C 0.001304000 -4.261283000 -0.675550000

C -0.000219000 -1.129911000 -2.883893000

C 0.002063000 -0.683266000 -4.244893000

C 0.000219000 1.129911000 -2.883893000

C -0.002063000 0.683266000 -4.244893000

C -0.004238000 2.455241000 -2.433332000

C 0.004238000 2.455241000 2.433332000

C -0.004238000 -2.455241000 2.433332000

C 0.004238000 -2.455241000 -2.433332000

C -0.011487000 3.519747000 -3.491484000

C 0.011487000 3.519747000 3.491484000

C -0.011487000 -3.519747000 3.491484000

C 0.011487000 -3.519747000 -3.491484000

H -0.005790000 -1.334505000 5.101770000

H 0.005790000 1.334505000 5.101770000

H 0.000791000 5.112644000 1.335376000

H -0.000791000 5.112644000 -1.335376000

H -0.005790000 1.334505000 -5.101770000

H 0.005790000 -1.334505000 -5.101770000

H 0.000791000 -5.112644000 -1.335376000

H -0.000791000 -5.112644000 1.335376000

C 1.179990000 3.895325000 -4.119254000

C -1.204411000 4.147471000 -3.864589000

C 1.146319000 4.880563000 -5.092757000

C -1.207613000 5.134374000 -4.847316000

H -2.137897000 5.611711000 -5.128125000

H -2.129455000 3.858711000 -3.382844000

C 1.204411000 4.147471000 3.864589000

C -1.179990000 3.895325000 4.119254000

C 1.207613000 5.134374000 4.847316000

C -1.146319000 4.880563000 5.092757000

H 2.129455000 3.858711000 3.382844000

H 2.137897000 5.611711000 5.128125000

C 1.179990000 -3.895325000 4.119254000

C -1.204411000 -4.147471000 3.864589000

C 1.146319000 -4.880563000 5.092757000

C -1.207613000 -5.134374000 4.847316000

H -2.137897000 -5.611711000 5.128125000

H -2.129455000 -3.858711000 3.382844000

C 1.204411000 -4.147471000 -3.864589000

C -1.179990000 -3.895325000 -4.119254000

C 1.207613000 -5.134374000 -4.847316000

C -1.146319000 -4.880563000 -5.092757000

H 2.129455000 -3.858711000 -3.382844000

H 2.137897000 -5.611711000 -5.128125000

C 0.024222000 -5.513826000 -5.475710000

C -0.024222000 5.513826000 -5.475710000

C 0.024222000 5.513826000 5.475710000

C -0.024222000 -5.513826000 5.475710000

H 0.000000000 0.000000000 1.091212000

H 0.000000000 0.000000000 -1.091212000

H -0.000229000 -6.277680000 6.240963000

H 0.000229000 6.277680000 6.240963000

H -0.000229000 6.277680000 -6.240963000

H 0.000229000 -6.277680000 -6.240963000

H 2.122435000 3.435331000 -3.853857000

H -2.122435000 -3.435331000 -3.853857000

H 2.122435000 -3.435331000 3.853857000

H -2.122435000 3.435331000 3.853857000

F -2.308477000 -5.238266000 -5.692265000

F 2.308477000 -5.238266000 5.692265000

F -2.308477000 5.238266000 5.692265000

F 2.308477000 5.238266000 -5.692265000

78

m-II m-4C6H4F-H2P

N -0.073716000 -2.054666000 -0.187982000

N -2.075440000 0.086732000 -0.154942000

N 0.125795000 2.017704000 -0.027879000

N 2.124774000 -0.126129000 0.002747000

C -1.200379000 -2.822041000 -0.221793000

C -0.861577000 -4.239496000 -0.176588000

C 0.969127000 -2.931846000 -0.140043000

C 0.486800000 -4.307716000 -0.125851000

C 2.849794000 -1.291957000 -0.049001000

C 4.230611000 -0.911566000 -0.050717000

C 2.960170000 0.963957000 0.040234000

C 4.297294000 0.452213000 0.003254000

C 1.249256000 2.782073000 0.085182000

C 0.903806000 4.193178000 0.209393000

C -0.920205000 2.891994000 0.002770000

C -0.444512000 4.261470000 0.158209000

C -2.797392000 1.255440000 -0.177957000

C -4.172343000 0.880454000 -0.319564000

C -2.907848000 -1.000555000 -0.266469000

C -4.239113000 -0.483337000 -0.373009000

C -2.524204000 -2.347600000 -0.281445000

C 2.334770000 -2.593480000 -0.098171000

C 2.575071000 2.309371000 0.095266000

C -2.283902000 2.555587000 -0.088882000

C -3.630086000 -3.355907000 -0.373991000

C 3.337319000 -3.708417000 -0.110327000

C 3.682494000 3.317367000 0.171933000

C -3.285372000 3.671399000 -0.097540000

H 5.184998000 1.060495000 0.008641000

H 5.055162000 -1.601512000 -0.097065000

H 1.100163000 -5.191193000 -0.069775000

H -1.563276000 -5.056472000 -0.169991000

H -5.122898000 -1.086995000 -0.485023000

H -4.992619000 1.574295000 -0.380734000

H -1.062799000 5.140225000 0.231239000

H 1.599951000 5.005613000 0.332674000

C -4.441974000 -3.616400000 0.734712000

C -3.867568000 -4.047856000 -1.566823000

C -5.456453000 -4.552950000 0.621949000

C -4.896886000 -4.981843000 -1.651284000

H -4.285087000 -3.107414000 1.676219000

H -5.072294000 -5.507056000 -2.581627000

H -3.245415000 -3.847390000 -2.429203000

C 3.596759000 -4.423025000 -1.285051000

C 4.029405000 -4.047405000 1.056871000

C 4.530260000 -5.456225000 -1.294360000

C 4.950225000 -5.081586000 1.018146000

H 3.067490000 -4.162476000 -2.192215000

H 4.724267000 -5.998238000 -2.211273000

H 3.850997000 -3.523514000 1.986296000

C 4.008323000 4.089891000 -0.947586000

C 4.404165000 3.500652000 1.356603000

C 5.034820000 5.014936000 -0.852097000

C 5.429406000 4.440748000 1.423723000

H 3.476130000 3.973792000 -1.882066000

H 5.975153000 4.577126000 2.348761000

H 4.152354000 2.910887000 2.228333000

C -3.446318000 4.478031000 -1.229573000

C -4.075066000 3.919181000 1.029990000

C -4.378722000 5.512216000 -1.235875000

C -4.992299000 4.956692000 0.995599000

H -2.841107000 4.288632000 -2.106384000

H -4.495651000 6.126176000 -2.119908000

H -3.974728000 3.322452000 1.926629000

C -5.166494000 5.764673000 -0.115571000

C -5.707326000 -5.246593000 -0.550155000

C 5.221123000 -5.799257000 -0.134853000

C 5.758289000 5.212509000 0.312269000

H 1.114812000 -0.075981000 -0.019925000

H -1.066830000 0.035269000 -0.099335000

H 6.550311000 5.948473000 0.338516000

H 5.949575000 -6.598399000 -0.115847000

H -6.511905000 -5.968195000 -0.589800000

H -5.896225000 6.562605000 -0.094946000

F 5.343037000 5.754929000 -1.945436000

F 5.610356000 -5.403323000 2.157768000

F -6.232584000 -4.799933000 1.705583000

F -5.747466000 5.189601000 2.097091000

78

m-III m-4C6H4F-H2P

N 0.000000000 0.000000000 2.040090000

N -0.118547000 2.100492000 0.000000000

N 0.000000000 0.000000000 -2.040090000

N 0.118547000 -2.100492000 0.000000000

C -0.088725000 1.083229000 2.863489000

C -0.052573000 0.673468000 4.262360000

C 0.088725000 -1.083229000 2.863489000

C 0.052573000 -0.673468000 4.262360000

C 0.216754000 -2.875700000 1.130061000

C 0.381074000 -4.226520000 0.683191000

C 0.216754000 -2.875700000 -1.130061000

C 0.381074000 -4.226520000 -0.683191000

C 0.088725000 -1.083229000 -2.863489000

C 0.052573000 -0.673468000 -4.262360000

C -0.088725000 1.083229000 -2.863489000

C -0.052573000 0.673468000 -4.262360000

C -0.216754000 2.875700000 -1.130061000

C -0.381074000 4.226520000 -0.683191000

C -0.216754000 2.875700000 1.130061000

C -0.381074000 4.226520000 0.683191000

C -0.192669000 2.426224000 2.456124000

C 0.192669000 -2.426224000 2.456124000

C 0.192669000 -2.426224000 -2.456124000

C -0.192669000 2.426224000 -2.456124000

C -0.301079000 3.479253000 3.518845000

C 0.301079000 -3.479253000 3.518845000

C 0.301079000 -3.479253000 -3.518845000

C -0.301079000 3.479253000 -3.518845000

H 0.496397000 -5.076044000 -1.333692000

H 0.496397000 -5.076044000 1.333692000

H 0.099976000 -1.330758000 5.114194000

H -0.099976000 1.330758000 5.114194000

H -0.496397000 5.076044000 1.333692000

H -0.496397000 5.076044000 -1.333692000

H -0.099976000 1.330758000 -5.114194000

H 0.099976000 -1.330758000 -5.114194000

C 0.802467000 4.279046000 3.832088000

C -1.502388000 3.679053000 4.207627000

C 0.676385000 5.245147000 4.816974000

C -1.599929000 4.659557000 5.191650000

H -2.536385000 4.805872000 5.714893000

H -2.360676000 3.065644000 3.966553000

C 1.502388000 -3.679053000 4.207627000

C -0.802467000 -4.279046000 3.832088000

C 1.599929000 -4.659557000 5.191650000

C -0.676385000 -5.245147000 4.816974000

H 2.360676000 -3.065644000 3.966553000

H 2.536385000 -4.805872000 5.714893000

C -0.802467000 -4.279046000 -3.832088000

C 1.502388000 -3.679053000 -4.207627000

C -0.676385000 -5.245147000 -4.816974000

C 1.599929000 -4.659557000 -5.191650000

H 2.536385000 -4.805872000 -5.714893000

H 2.360676000 -3.065644000 -3.966553000

C -1.502388000 3.679053000 -4.207627000

C 0.802467000 4.279046000 -3.832088000

C -1.599929000 4.659557000 -5.191650000

C 0.676385000 5.245147000 -4.816974000

H -2.360676000 3.065644000 -3.966553000

H -2.536385000 4.805872000 -5.714893000

C -0.503998000 5.458009000 -5.509209000

C -0.503998000 5.458009000 5.509209000

C 0.503998000 -5.458009000 5.509209000

C 0.503998000 -5.458009000 -5.509209000

H 0.010932000 -1.094678000 0.000000000

H -0.010932000 1.094678000 0.000000000

H 0.553958000 -6.225158000 -6.269882000

H 0.553958000 -6.225158000 6.269882000

H -0.553958000 6.225158000 6.269882000

H -0.553958000 6.225158000 -6.269882000

H 1.749572000 4.150513000 3.325494000

H 1.749572000 4.150513000 -3.325494000

H -1.749572000 -4.150513000 -3.325494000

H -1.749572000 -4.150513000 3.325494000

F -1.754934000 -6.010738000 5.114422000

F 1.754934000 6.010738000 5.114422000

F 1.754934000 6.010738000 -5.114422000

F -1.754934000 -6.010738000 -5.114422000

78

m-IV m-4C6H4F-H2P

N -2.031864000 0.179965000 0.000000000

N 0.000000000 0.000000000 2.103378000

N 2.031864000 -0.179965000 0.000000000

N 0.000000000 0.000000000 -2.103378000

C -2.854758000 0.211964000 1.086779000

C -4.252814000 0.261290000 0.675521000

C -2.854758000 0.211964000 -1.086779000

C -4.252814000 0.261290000 -0.675521000

C -1.127152000 0.081462000 -2.884547000

C -0.681240000 0.052126000 -4.245379000

C 1.127152000 -0.081462000 -2.884547000

C 0.681240000 -0.052126000 -4.245379000

C 2.854758000 -0.211964000 -1.086779000

C 4.252814000 -0.261290000 -0.675521000

C 2.854758000 -0.211964000 1.086779000

C 4.252814000 -0.261290000 0.675521000

C 1.127152000 -0.081462000 2.884547000

C 0.681240000 -0.052126000 4.245379000

C -1.127152000 0.081462000 2.884547000

C -0.681240000 0.052126000 4.245379000

C -2.449305000 0.178666000 2.433890000

C -2.449305000 0.178666000 -2.433890000

C 2.449305000 -0.178666000 -2.433890000

C 2.449305000 -0.178666000 2.433890000

C -3.511529000 0.250676000 3.490871000

C -3.511529000 0.250676000 -3.490871000

C 3.511529000 -0.250676000 -3.490871000

C 3.511529000 -0.250676000 3.490871000

H 1.329628000 -0.104631000 -5.102685000

H -1.329628000 0.104631000 -5.102685000

H -5.104238000 0.279375000 -1.334894000

H -5.104238000 0.279375000 1.334894000

H -1.329628000 0.104631000 5.102685000

H 1.329628000 -0.104631000 5.102685000

H 5.104238000 -0.279375000 1.334894000

H 5.104238000 -0.279375000 -1.334894000

C -3.907919000 -0.904642000 4.171749000

C -4.117877000 1.470053000 3.811069000

C -4.891033000 -0.809957000 5.143236000

C -5.102461000 1.534874000 4.793809000

H -5.561613000 2.485437000 5.034132000

H -3.812526000 2.367649000 3.289379000

C -4.117877000 1.470053000 -3.811069000

C -3.907919000 -0.904642000 -4.171749000

C -5.102461000 1.534874000 -4.793809000

C -4.891033000 -0.809957000 -5.143236000

H -3.812526000 2.367649000 -3.289379000

H -5.561613000 2.485437000 -5.034132000

C 3.907919000 0.904642000 -4.171749000

C 4.117877000 -1.470053000 -3.811069000

C 4.891033000 0.809957000 -5.143236000

C 5.102461000 -1.534874000 -4.793809000

H 5.561613000 -2.485437000 -5.034132000

H 3.812526000 -2.367649000 -3.289379000

C 4.117877000 -1.470053000 3.811069000

C 3.907919000 0.904642000 4.171749000

C 5.102461000 -1.534874000 4.793809000

C 4.891033000 0.809957000 5.143236000

H 3.812526000 -2.367649000 3.289379000

H 5.561613000 -2.485437000 5.034132000

C 5.502329000 -0.387713000 5.474567000

C -5.502329000 0.387713000 5.474567000

C -5.502329000 0.387713000 -5.474567000

C 5.502329000 -0.387713000 -5.474567000

H 0.000000000 0.000000000 -1.091917000

H 0.000000000 0.000000000 1.091917000

H 6.265206000 -0.411562000 -6.240786000

H -6.265206000 0.411562000 -6.240786000

H -6.265206000 0.411562000 6.240786000

H 6.265206000 -0.411562000 6.240786000

H -3.466797000 -1.866557000 3.947435000

H 3.466797000 1.866557000 3.947435000

H 3.466797000 1.866557000 -3.947435000

H -3.466797000 -1.866557000 -3.947435000

F -5.269373000 -1.937851000 -5.793282000

F -5.269373000 -1.937851000 5.793282000

F 5.269373000 1.937851000 5.793282000

F 5.269373000 1.937851000 -5.793282000

78

m-V m-4C6H4F-H2P

N -2.040143000 0.000000000 -0.210723000

N 0.000000000 2.104423000 -0.178295000

N 2.040143000 0.000000000 -0.210723000

N 0.000000000 -2.104423000 -0.178295000

C -2.862546000 1.086910000 -0.170042000

C -4.258644000 0.675520000 -0.083154000

C -2.862546000 -1.086910000 -0.170042000

C -4.258644000 -0.675520000 -0.083154000

C -1.130222000 -2.884667000 -0.215669000

C -0.683227000 -4.243399000 -0.288000000

C 1.130222000 -2.884667000 -0.215669000

C 0.683227000 -4.243399000 -0.288000000

C 2.862546000 -1.086910000 -0.170042000

C 4.258644000 -0.675520000 -0.083154000

C 2.862546000 1.086910000 -0.170042000

C 4.258644000 0.675520000 -0.083154000

C 1.130222000 2.884667000 -0.215669000

C 0.683227000 4.243399000 -0.288000000

C -1.130222000 2.884667000 -0.215669000

C -0.683227000 4.243399000 -0.288000000

C -2.456389000 2.434404000 -0.195196000

C -2.456389000 -2.434404000 -0.195196000

C 2.456389000 -2.434404000 -0.195196000

C 2.456389000 2.434404000 -0.195196000

C -3.520568000 3.490588000 -0.205337000

C -3.520568000 -3.490588000 -0.205337000

C 3.520568000 -3.490588000 -0.205337000

C 3.520568000 3.490588000 -0.205337000

H 1.333216000 -5.099335000 -0.341739000

H -1.333216000 -5.099335000 -0.341739000

H -5.108011000 -1.334306000 -0.016596000

H -5.108011000 1.334306000 -0.016596000

H -1.333216000 5.099335000 -0.341739000

H 1.333216000 5.099335000 -0.341739000

H 5.108011000 1.334306000 -0.016596000

H 5.108011000 -1.334306000 -0.016596000

C -3.773819000 4.248089000 0.942861000

C -4.272700000 3.735477000 -1.359635000

C -4.762720000 5.217479000 0.906181000

C -5.258616000 4.718759000 -1.367586000

H -3.218889000 4.083354000 1.856660000

H -5.830320000 4.900659000 -2.268823000

H -4.078368000 3.155469000 -2.252262000

C -4.272700000 -3.735477000 -1.359635000

C -3.773819000 -4.248089000 0.942861000

C -5.258616000 -4.718759000 -1.367586000

C -4.762720000 -5.217479000 0.906181000

H -4.078368000 -3.155469000 -2.252262000

H -5.830320000 -4.900659000 -2.268823000

H -3.218889000 -4.083354000 1.856660000

C 3.773819000 -4.248089000 0.942861000

C 4.272700000 -3.735477000 -1.359635000

C 4.762720000 -5.217479000 0.906181000

C 5.258616000 -4.718759000 -1.367586000

H 3.218889000 -4.083354000 1.856660000

H 5.830320000 -4.900659000 -2.268823000

H 4.078368000 -3.155469000 -2.252262000

C 4.272700000 3.735477000 -1.359635000

C 3.773819000 4.248089000 0.942861000

C 5.258616000 4.718759000 -1.367586000

C 4.762720000 5.217479000 0.906181000

H 4.078368000 3.155469000 -2.252262000

H 5.830320000 4.900659000 -2.268823000

H 3.218889000 4.083354000 1.856660000

C 5.516304000 5.474882000 -0.226856000

C -5.516304000 5.474882000 -0.226856000

C -5.516304000 -5.474882000 -0.226856000

C 5.516304000 -5.474882000 -0.226856000

H 0.000000000 -1.093103000 -0.161366000

H 0.000000000 1.093103000 -0.161366000

H 6.277435000 -6.242943000 -0.207064000

H -6.277435000 -6.242943000 -0.207064000

H -6.277435000 6.242943000 -0.207064000

H 6.277435000 6.242943000 -0.207064000

F 5.001753000 -5.940851000 2.027407000

F -5.001753000 -5.940851000 2.027407000

F -5.001753000 5.940851000 2.027407000

F 5.001753000 5.940851000 2.027407000

78

o-I o-4C6H4F-H2P

N -2.038536000 0.000000000 0.000000000

N 0.000000000 -2.101756000 0.000000000

N 2.038536000 0.000000000 0.000000000

N 0.000000000 2.101756000 0.000000000

C -2.861603000 -1.086046000 -0.005189000

C -4.260870000 -0.675478000 -0.003311000

C -2.861603000 1.086046000 0.005189000

C -4.260870000 0.675478000 0.003311000

C -1.129031000 2.882691000 0.004326000

C -0.683118000 4.243718000 0.004537000

C 1.129031000 2.882691000 -0.004326000

C 0.683120000 4.243718000 -0.004537000

C 2.861603000 1.086046000 -0.005189000

C 4.260870000 0.675478000 -0.003311000

C 2.861603000 -1.086046000 0.005188000

C 4.260870000 -0.675478000 0.003311000

C 1.129031000 -2.882691000 0.004326000

C 0.683119000 -4.243718000 0.004537000

C -1.129031000 -2.882691000 -0.004326000

C -0.683119000 -4.243718000 -0.004537000

C -2.453285000 -2.431601000 -0.009015000

C -2.453285000 2.431601000 0.009015000

C 2.453285000 2.431602000 -0.009015000

C 2.453285000 -2.431601000 0.009015000

C -3.516888000 -3.488029000 -0.030654000

C -3.516888000 3.488029000 0.030654000

C 3.516887000 3.488030000 -0.030654000

C 3.516888000 -3.488029000 0.030654000

H 1.334960000 5.100411000 -0.010101000

H -1.334958000 5.100411000 0.010101000

H -5.112324000 1.335519000 0.006311000

H -5.112324000 -1.335517000 -0.006311000

H -1.334960000 -5.100411000 -0.010101000

H 1.334958000 -5.100411000 0.010101000

H 5.112324000 -1.335519000 0.006311000

H 5.112324000 1.335517000 -0.006311000

C -3.991547000 -4.071845000 1.141912000

C -4.080564000 -3.933051000 -1.231848000

C -4.975824000 -5.048403000 1.155220000

C -5.069775000 -4.911973000 -1.250106000

H -5.488320000 -5.236923000 -2.193855000

H -3.730524000 -3.496445000 -2.158835000

C -4.080564000 3.933051000 1.231848000

C -3.991546000 4.071845000 -1.141912000

C -5.069774000 4.911975000 1.250106000

C -4.975822000 5.048405000 -1.155220000

H -3.730524000 3.496446000 2.158835000

H -5.488318000 5.236925000 2.193855000

C 3.991548000 4.071846000 1.141912000

C 4.080564000 3.933051000 -1.231848000

C 4.975824000 5.048403000 1.155220000

C 5.069775000 4.911974000 -1.250106000

H 5.488320000 5.236923000 -2.193855000

H 3.730524000 3.496446000 -2.158835000

C 4.080564000 -3.933051000 1.231847000

C 3.991547000 -4.071845000 -1.141912000

C 5.069775000 -4.911975000 1.250106000

C 4.975822000 -5.048405000 -1.155220000

H 3.730524000 -3.496445000 2.158835000

H 5.488318000 -5.236925000 2.193855000

C 5.517763000 -5.469941000 0.054931000

C -5.517765000 -5.469939000 -0.054931000

C -5.517764000 5.469941000 0.054931000

C 5.517765000 5.469939000 -0.054931000

H 0.000000000 1.090325000 0.000000000

H 0.000000000 -1.090325000 0.000000000

H 6.287282000 6.231397000 -0.061010000

H -6.287280000 6.231399000 0.061011000

H -6.287282000 -6.231397000 -0.061010000

H 6.287280000 -6.231399000 0.061010000

H 5.301523000 -5.459137000 -2.101576000

H 5.301525000 5.459135000 2.101576000

H -5.301524000 5.459137000 -2.101576000

H -5.301525000 -5.459135000 2.101576000

F 3.476002000 3.672830000 2.328547000

F 3.476001000 -3.672831000 -2.328547000

F -3.476001000 -3.672831000 2.328547000

F -3.476002000 3.672830000 -2.328547000

78

o-II o-4C6H4F-H2P

N 0.303866000 -2.012810000 -0.043897000

N -2.071045000 -0.303926000 -0.142723000

N -0.287724000 2.020132000 -0.165344000

N 2.086522000 0.311385000 -0.047307000

C -0.650200000 -2.985903000 -0.047150000

C -0.040586000 -4.308905000 0.023308000

C 1.497294000 -2.667117000 0.021604000

C 1.295056000 -4.110417000 0.066123000

C 3.022618000 -0.691481000 0.005051000

C 4.304240000 -0.052171000 0.021176000

C 2.695247000 1.541740000 -0.062189000

C 4.106166000 1.298871000 -0.023130000

C 0.666066000 2.993062000 -0.138144000

C 0.055276000 4.317147000 -0.144036000

C -1.482359000 2.675439000 -0.193192000

C -1.280841000 4.119701000 -0.177630000

C -3.006288000 0.698277000 -0.215942000

C -4.285190000 0.057672000 -0.286000000

C -2.678058000 -1.535111000 -0.160936000

C -4.086585000 -1.293599000 -0.253041000

C -2.039792000 -2.779238000 -0.109513000

C 2.768569000 -2.066532000 0.041618000

C 2.056698000 2.785842000 -0.102438000

C -2.753435000 2.074510000 -0.229419000

C -2.927917000 -3.986309000 -0.139848000

C 3.967679000 -2.963071000 0.121913000

C 2.946326000 3.992261000 -0.114278000

C -3.951478000 2.972135000 -0.302327000

H 4.859220000 2.068136000 -0.027358000

H 5.245974000 -0.572094000 0.061841000

H 2.071531000 -4.855071000 0.123507000

H -0.569169000 -5.247427000 0.040160000

H -4.837696000 -2.063789000 -0.291693000

H -5.225816000 0.576410000 -0.356497000

H -2.057994000 4.865673000 -0.182931000

H 0.583064000 5.255927000 -0.117391000

C -3.542910000 -4.471640000 1.012482000

C -3.176348000 -4.680906000 -1.329340000

C -4.366848000 -5.586946000 1.016708000

C -3.999332000 -5.802916000 -1.356217000

H -4.174150000 -6.320211000 -2.290727000

H -2.711005000 -4.326235000 -2.240445000

C 4.488639000 -3.378331000 1.352636000

C 4.615102000 -3.422078000 -1.023083000

C 5.600359000 -4.212624000 1.425261000

C 5.723919000 -4.253626000 -0.982287000

H 4.004903000 -3.036854000 2.259205000

H 5.981425000 -4.518990000 2.390844000

C 3.469097000 4.528336000 1.060840000

C 3.289330000 4.634891000 -1.309384000

C 4.291131000 5.644831000 1.081904000

C 4.113145000 5.756594000 -1.319810000

H 4.362503000 6.232905000 -2.259180000

H 2.897974000 4.239281000 -2.238242000

C -4.374588000 3.529079000 -1.514767000

C -4.695065000 3.294341000 0.831362000

C -5.485651000 4.364511000 -1.581408000

C -5.805267000 4.124421000 0.796054000

H -3.815725000 3.295499000 -2.412296000

H -5.790583000 4.780204000 -2.533091000

C -6.201631000 4.662491000 -0.424189000

C -4.595189000 -6.256211000 -0.181471000

C 6.218277000 -4.650704000 0.256197000

C 4.614260000 6.262100000 -0.122379000

H 1.086272000 0.164149000 -0.076154000

H -1.071950000 -0.156198000 -0.088597000

H 5.254918000 7.134773000 -0.122144000

H 7.083086000 -5.300144000 0.304614000

H -5.236017000 -7.128670000 -0.194137000

H -7.066442000 5.312268000 -0.467654000

H -6.335831000 4.337622000 1.714421000

H 4.660382000 6.012409000 2.030007000

H 6.178895000 -4.575596000 -1.909493000

H -4.810790000 -5.913395000 1.947679000

F 3.163817000 3.941965000 2.242006000

F -4.322225000 2.783213000 2.027577000

F -3.329213000 -3.835319000 2.187749000

F 4.147405000 -3.045252000 -2.236604000

78

o-III o-4C6H4F-H2P

N 0.000000000 0.000000000 2.038976000

N -0.096121000 2.099771000 0.000000000

N 0.000000000 0.000000000 -2.038976000

N 0.096121000 -2.099771000 0.000000000

C -0.062814000 1.084300000 2.861988000

C -0.038733000 0.674394000 4.261244000

C 0.062814000 -1.084300000 2.861988000

C 0.038733000 -0.674394000 4.261244000

C 0.161112000 -2.878053000 1.129036000

C 0.270704000 -4.234614000 0.683107000

C 0.161112000 -2.878053000 -1.129036000

C 0.270704000 -4.234614000 -0.683107000

C 0.062814000 -1.084300000 -2.861988000

C 0.038733000 -0.674394000 -4.261244000

C -0.062814000 1.084300000 -2.861988000

C -0.038733000 0.674394000 -4.261244000

C -0.161112000 2.878053000 -1.129036000

C -0.270704000 4.234614000 -0.683107000

C -0.161112000 2.878053000 1.129036000

C -0.270704000 4.234614000 0.683107000

C -0.140641000 2.427642000 2.453471000

C 0.140641000 -2.427642000 2.453471000

C 0.140641000 -2.427642000 -2.453471000

C -0.140641000 2.427642000 -2.453471000

C -0.227492000 3.480626000 3.516920000

C 0.227492000 -3.480626000 3.516920000

C 0.227492000 -3.480626000 -3.516920000

C -0.227492000 3.480626000 -3.516920000

H 0.344271000 -5.088231000 -1.334863000

H 0.344271000 -5.088231000 1.334863000

H 0.075469000 -1.333284000 5.112756000

H -0.075469000 1.333284000 5.112756000

H -0.344271000 5.088231000 1.334863000

H -0.344271000 5.088231000 -1.334863000

H -0.075469000 1.333284000 -5.112756000

H 0.075469000 -1.333284000 -5.112756000

C 0.902150000 4.161931000 3.965328000

C -1.449004000 3.824273000 4.107447000

C 0.854862000 5.138621000 4.948491000

C -1.527748000 4.800779000 5.096017000

H -2.486020000 5.046344000 5.535188000

H -2.343547000 3.310388000 3.778524000

C 1.449004000 -3.824273000 4.107447000

C -0.902150000 -4.161931000 3.965328000

C 1.527748000 -4.800779000 5.096017000

C -0.854862000 -5.138621000 4.948491000

H 2.343547000 -3.310388000 3.778524000

H 2.486020000 -5.046344000 5.535188000

C -0.902150000 -4.161931000 -3.965328000

C 1.449004000 -3.824273000 -4.107447000

C -0.854862000 -5.138621000 -4.948491000

C 1.527748000 -4.800779000 -5.096017000

H 2.486020000 -5.046344000 -5.535188000

H 2.343547000 -3.310388000 -3.778524000

C -1.449004000 3.824273000 -4.107447000

C 0.902150000 4.161931000 -3.965328000

C -1.527748000 4.800779000 -5.096017000

C 0.854862000 5.138621000 -4.948491000

H -2.343547000 3.310388000 -3.778524000

H -2.486020000 5.046344000 -5.535188000

C -0.374134000 5.458557000 -5.516779000

C -0.374134000 5.458557000 5.516779000

C 0.374134000 -5.458557000 5.516779000

C 0.374134000 -5.458557000 -5.516779000

H 0.014862000 -1.091579000 0.000000000

H -0.014862000 1.091579000 0.000000000

H 0.427198000 -6.218841000 -6.285648000

H 0.427198000 -6.218841000 6.285648000

H -0.427198000 6.218841000 6.285648000

H -0.427198000 6.218841000 -6.285648000

H 1.770444000 5.627691000 -5.253257000

H -1.770444000 -5.627691000 -5.253257000

H -1.770444000 -5.627691000 5.253257000

H 1.770444000 5.627691000 5.253257000

F -2.106567000 -3.861538000 -3.425534000

F 2.106567000 3.861538000 -3.425534000

F 2.106567000 3.861538000 3.425534000

F -2.106567000 -3.861538000 3.425534000

78

o-IV o-4C6H4F-H2P

N -2.035387000 0.121273000 0.000000000

N 0.000000000 0.000000000 2.101825000

N 2.035387000 -0.121273000 0.000000000

N 0.000000000 0.000000000 -2.101825000

C -2.857968000 0.148309000 1.086151000

C -4.256494000 0.192844000 0.675510000

C -2.857968000 0.148309000 -1.086151000

C -4.256494000 0.192844000 -0.675510000

C -1.127443000 0.059613000 -2.882771000

C -0.682019000 0.038100000 -4.243740000

C 1.127443000 -0.059613000 -2.882771000

C 0.682019000 -0.038100000 -4.243740000

C 2.857968000 -0.148309000 -1.086151000

C 4.256494000 -0.192844000 -0.675510000

C 2.857968000 -0.148309000 1.086151000

C 4.256494000 -0.192844000 0.675510000

C 1.127443000 -0.059613000 2.882771000

C 0.682019000 -0.038100000 4.243740000

C -1.127443000 0.059613000 2.882771000

C -0.682019000 0.038100000 4.243740000

C -2.450036000 0.128263000 2.431856000

C -2.450036000 0.128263000 -2.431856000

C 2.450036000 -0.128263000 -2.431856000

C 2.450036000 -0.128263000 2.431856000

C -3.511954000 0.193720000 3.487928000

C -3.511954000 0.193720000 -3.487928000

C 3.511954000 -0.193720000 -3.487928000

C 3.511954000 -0.193720000 3.487928000

H 1.332586000 -0.076215000 -5.100562000

H -1.332586000 0.076215000 -5.100562000

H -5.107784000 0.213394000 -1.335403000

H -5.107784000 0.213394000 1.335403000

H -1.332586000 0.076215000 5.100562000

H 1.332586000 -0.076215000 5.100562000

H 5.107784000 -0.213394000 1.335403000

H 5.107784000 -0.213394000 -1.335403000

C -4.007833000 -0.955706000 4.099742000

C -4.053477000 1.415274000 3.904346000

C -4.991807000 -0.927464000 5.076321000

C -5.041344000 1.475190000 4.882893000

H -5.441681000 2.434030000 5.185894000

H -3.686059000 2.325074000 3.446401000

C -4.053477000 1.415274000 -3.904346000

C -4.007833000 -0.955706000 -4.099742000

C -5.041344000 1.475190000 -4.882893000

C -4.991807000 -0.927464000 -5.076321000

H -3.686059000 2.325074000 -3.446401000

H -5.441681000 2.434030000 -5.185894000

C 4.007833000 0.955706000 -4.099742000

C 4.053477000 -1.415274000 -3.904346000

C 4.991807000 0.927464000 -5.076321000

C 5.041344000 -1.475190000 -4.882893000

H 5.441681000 -2.434030000 -5.185894000

H 3.686059000 -2.325074000 -3.446401000

C 4.053477000 -1.415274000 3.904346000

C 4.007833000 0.955706000 4.099742000

C 5.041344000 -1.475190000 4.882893000

C 4.991807000 0.927464000 5.076321000

H 3.686059000 -2.325074000 3.446401000

H 5.441681000 -2.434030000 5.185894000

C 5.511032000 -0.302103000 5.469187000

C -5.511032000 0.302103000 5.469187000

C -5.511032000 0.302103000 -5.469187000

C 5.511032000 -0.302103000 -5.469187000

H 0.000000000 0.000000000 -1.090407000

H 0.000000000 0.000000000 1.090407000

H 6.279834000 -0.340452000 -6.230421000

H -6.279834000 0.340452000 -6.230421000

H -6.279834000 0.340452000 6.230421000

H 6.279834000 -0.340452000 6.230421000

H 5.335286000 1.857718000 5.508772000

H 5.335286000 1.857718000 -5.508772000

H -5.335286000 -1.857718000 -5.508772000

H -5.335286000 -1.857718000 5.508772000

F 3.515336000 2.160820000 -3.728731000

F 3.515336000 2.160820000 3.728731000

F -3.515336000 -2.160820000 3.728731000

F -3.515336000 -2.160820000 -3.728731000

78

o-V o-4C6H4F-H2P

N -2.039213000 0.000000000 -0.212609000

N 0.000000000 2.102114000 -0.196416000

N 2.039213000 0.000000000 -0.212609000

N 0.000000000 -2.102114000 -0.196416000

C -2.861827000 1.086230000 -0.187666000

C -4.260164000 0.675529000 -0.138582000

C -2.861827000 -1.086230000 -0.187666000

C -4.260164000 -0.675529000 -0.138582000

C -1.129035000 -2.882750000 -0.216823000

C -0.683069000 -4.243042000 -0.257926000

C 1.129035000 -2.882750000 -0.216823000

C 0.683069000 -4.243042000 -0.257926000

C 2.861827000 -1.086230000 -0.187666000

C 4.260164000 -0.675529000 -0.138582000

C 2.861827000 1.086230000 -0.187666000

C 4.260164000 0.675529000 -0.138582000

C 1.129035000 2.882750000 -0.216823000

C 0.683069000 4.243042000 -0.257926000

C -1.129035000 2.882750000 -0.216823000

C -0.683069000 4.243042000 -0.257926000

C -2.453574000 2.432038000 -0.203739000

C -2.453574000 -2.432038000 -0.203739000

C 2.453574000 -2.432038000 -0.203739000

C 2.453574000 2.432038000 -0.203739000

C -3.517663000 3.487547000 -0.218158000

C -3.517663000 -3.487547000 -0.218158000

C 3.517663000 -3.487547000 -0.218158000

C 3.517663000 3.487547000 -0.218158000

H 1.334617000 -5.099518000 -0.285680000

H -1.334617000 -5.099518000 -0.285680000

H -5.110935000 -1.335253000 -0.100529000

H -5.110935000 1.335253000 -0.100529000

H -1.334617000 5.099518000 -0.285680000

H 1.334617000 5.099518000 -0.285680000

H 5.110935000 1.335253000 -0.100529000

H 5.110935000 -1.335253000 -0.100529000

C -3.917881000 4.139380000 0.946718000

C -4.158508000 3.863152000 -1.404464000

C -4.901276000 5.116861000 0.965690000

C -5.148043000 4.841717000 -1.416665000

H -5.625988000 5.112811000 -2.349175000

H -3.867349000 3.373291000 -2.325188000

C -4.158508000 -3.863152000 -1.404464000

C -3.917881000 -4.139380000 0.946718000

C -5.148043000 -4.841717000 -1.416665000

C -4.901276000 -5.116861000 0.965690000

H -3.867349000 -3.373291000 -2.325188000

H -5.625988000 -5.112811000 -2.349175000

C 3.917881000 -4.139380000 0.946718000

C 4.158508000 -3.863152000 -1.404464000

C 4.901276000 -5.116861000 0.965690000

C 5.148043000 -4.841717000 -1.416665000

H 5.625988000 -5.112811000 -2.349175000

H 3.867349000 -3.373291000 -2.325188000

C 4.158508000 3.863152000 -1.404464000

C 3.917881000 4.139380000 0.946718000

C 5.148043000 4.841717000 -1.416665000

C 4.901276000 5.116861000 0.965690000

H 3.867349000 3.373291000 -2.325188000

H 5.625988000 5.112811000 -2.349175000

C 5.519750000 5.469082000 -0.229732000

C -5.519750000 5.469082000 -0.229732000

C -5.519750000 -5.469082000 -0.229732000

C 5.519750000 -5.469082000 -0.229732000

H 0.000000000 -1.090948000 -0.174726000

H 0.000000000 1.090948000 -0.174726000

H 6.289295000 -6.230530000 -0.230791000

H -6.289295000 -6.230530000 -0.230791000

H -6.289295000 6.230530000 -0.230791000

H 6.289295000 6.230530000 -0.230791000

H 5.167708000 5.581022000 1.905859000

H 5.167708000 -5.581022000 1.905859000

H -5.167708000 -5.581022000 1.905859000

H -5.167708000 5.581022000 1.905859000

F 3.329808000 -3.807369000 2.119171000

F 3.329808000 3.807369000 2.119171000

F -3.329808000 3.807369000 2.119171000

F -3.329808000 -3.807369000 2.119171000

78

p-I p-4C6H4Br-H2P

N 2.040634000 0.000000000 -0.005640000

N 0.000000000 2.104692000 -0.039066000

N -2.040634000 0.000000000 -0.005640000

N 0.000000000 -2.104692000 -0.039066000

C 2.862619000 1.087131000 -0.051689000

C 4.257805000 0.675584000 -0.150590000

C 2.862619000 -1.087131000 -0.051689000

C 4.257805000 -0.675584000 -0.150590000

C 1.130442000 -2.884475000 0.005798000

C 0.683315000 -4.242260000 0.091809000

C -1.130442000 -2.884475000 0.005798000

C -0.683315000 -4.242260000 0.091809000

C -2.862619000 -1.087131000 -0.051689000

C -4.257805000 -0.675584000 -0.150590000

C -2.862619000 1.087131000 -0.051689000

C -4.257805000 0.675584000 -0.150590000

C -1.130442000 2.884475000 0.005798000

C -0.683315000 4.242260000 0.091809000

C 1.130442000 2.884475000 0.005798000

C 0.683315000 4.242260000 0.091809000

C 2.457348000 2.435217000 -0.019993000

C 2.457348000 -2.435217000 -0.019993000

C -2.457348000 -2.435217000 -0.019993000

C -2.457348000 2.435217000 -0.019993000

C 3.520251000 3.491046000 -0.009938000

C 3.520251000 -3.491046000 -0.009938000

C -3.520251000 -3.491046000 -0.009938000

C -3.520251000 3.491046000 -0.009938000

H -1.333149000 -5.097496000 0.157293000

H 1.333149000 -5.097496000 0.157293000

H 5.106989000 -1.333569000 -0.226582000

H 5.106989000 1.333569000 -0.226582000

H 1.333149000 5.097496000 0.157293000

H -1.333149000 5.097496000 0.157293000

H -5.106989000 1.333569000 -0.226582000

H -5.106989000 -1.333569000 -0.226582000

C 3.761507000 4.277976000 -1.140577000

C 4.295607000 3.714426000 1.132403000

C 4.749203000 5.259617000 -1.138670000

C 5.284438000 4.694499000 1.152174000

H 3.177500000 4.115737000 -2.037926000

H 4.930034000 5.855691000 -2.022492000

H 5.873037000 4.859872000 2.043988000

H 4.121233000 3.118848000 2.019686000

C 4.295607000 -3.714426000 1.132403000

C 3.761507000 -4.277976000 -1.140577000

C 5.284438000 -4.694499000 1.152174000

C 4.749203000 -5.259617000 -1.138670000

H 4.121233000 -3.118848000 2.019686000

H 5.873037000 -4.859872000 2.043988000

H 4.930034000 -5.855691000 -2.022492000

H 3.177500000 -4.115737000 -2.037926000

C -3.761507000 -4.277976000 -1.140577000

C -4.295607000 -3.714426000 1.132403000

C -4.749203000 -5.259617000 -1.138670000

C -5.284438000 -4.694499000 1.152174000

H -3.177500000 -4.115737000 -2.037926000

H -4.930034000 -5.855691000 -2.022492000

H -5.873037000 -4.859872000 2.043988000

H -4.121233000 -3.118848000 2.019686000

C -4.295607000 3.714426000 1.132403000

C -3.761507000 4.277976000 -1.140577000

C -5.284438000 4.694499000 1.152174000

C -4.749203000 5.259617000 -1.138670000

H -4.121233000 3.118848000 2.019686000

H -5.873037000 4.859872000 2.043988000

H -4.930034000 5.855691000 -2.022492000

H -3.177500000 4.115737000 -2.037926000

C -5.502664000 5.459531000 0.012202000

C 5.502664000 5.459531000 0.012202000

C 5.502664000 -5.459531000 0.012202000

C -5.502664000 -5.459531000 0.012202000

H 0.000000000 -1.093452000 -0.059999000

H 0.000000000 1.093452000 -0.059999000

Br 6.860652000 -6.807342000 0.027284000

Br -6.860652000 -6.807342000 0.027284000

Br -6.860652000 6.807342000 0.027284000

Br 6.860652000 6.807342000 0.027284000

78

p-II p-4C6H4Br-H2P

N 0.000000000 0.000000000 2.040719000

N 2.102714000 0.071998000 0.000000000

N 0.000000000 0.000000000 -2.040719000

N -2.102714000 -0.071998000 0.000000000

C 1.087039000 0.008040000 2.864003000

C 0.675517000 0.008214000 4.262770000

C -1.087039000 -0.008040000 2.864003000

C -0.675517000 -0.008214000 4.262770000

C -2.883353000 -0.037221000 1.130254000

C -4.242961000 0.015908000 0.683258000

C -2.883353000 -0.037221000 -1.130254000

C -4.242961000 0.015908000 -0.683258000

C -1.087039000 -0.008040000 -2.864003000

C -0.675517000 -0.008214000 -4.262770000

C 1.087039000 0.008040000 -2.864003000

C 0.675517000 0.008214000 -4.262770000

C 2.883353000 0.037221000 -1.130254000

C 4.242961000 -0.015908000 -0.683258000

C 2.883353000 0.037221000 1.130254000

C 4.242961000 -0.015908000 0.683258000

C 2.434512000 0.022014000 2.457114000

C -2.434512000 -0.022014000 2.457114000

C -2.434512000 -0.022014000 -2.457114000

C 2.434512000 0.022014000 -2.457114000

C 3.493158000 0.007798000 3.518316000

C -3.493158000 -0.007798000 3.518316000

C -3.493158000 -0.007798000 -3.518316000

C 3.493158000 0.007798000 -3.518316000

H -5.098961000 0.064339000 -1.333675000

H -5.098961000 0.064339000 1.333675000

H -1.333642000 -0.021596000 5.115140000

H 1.333642000 0.021596000 5.115140000

H 5.098961000 -0.064339000 1.333675000

H 5.098961000 -0.064339000 -1.333675000

H 1.333642000 0.021596000 -5.115140000

H -1.333642000 -0.021596000 -5.115140000

C 3.784308000 -1.163778000 4.223989000

C 4.215388000 1.165186000 3.824601000

C 4.767783000 -1.185703000 5.209570000

C 5.200238000 1.160948000 4.809282000

H 3.239042000 -2.071678000 3.998337000

H 4.985520000 -2.099534000 5.744952000

H 5.746928000 2.064735000 5.040455000

H 4.000785000 2.084161000 3.293437000

C -3.784308000 1.163778000 4.223989000

C -4.215388000 -1.165186000 3.824601000

C -4.767783000 1.185703000 5.209570000

C -5.200238000 -1.160948000 4.809282000

H -3.239042000 2.071678000 3.998337000

H -4.985520000 2.099534000 5.744952000

H -5.746928000 -2.064735000 5.040455000

H -4.000785000 -2.084161000 3.293437000

C -4.215388000 -1.165186000 -3.824601000

C -3.784308000 1.163778000 -4.223989000

C -5.200238000 -1.160948000 -4.809282000

C -4.767783000 1.185703000 -5.209570000

H -4.000785000 -2.084161000 -3.293437000

H -5.746928000 -2.064735000 -5.040455000

H -4.985520000 2.099534000 -5.744952000

H -3.239042000 2.071678000 -3.998337000

C 4.215388000 1.165186000 -3.824601000

C 3.784308000 -1.163778000 -4.223989000

C 5.200238000 1.160948000 -4.809282000

C 4.767783000 -1.185703000 -5.209570000

H 4.000785000 2.084161000 -3.293437000

H 5.746928000 2.064735000 -5.040455000

H 4.985520000 -2.099534000 -5.744952000

H 3.239042000 -2.071678000 -3.998337000

C 5.467869000 -0.018851000 -5.493736000

C 5.467869000 -0.018851000 5.493736000

C -5.467869000 0.018851000 5.493736000

C -5.467869000 0.018851000 -5.493736000

H -1.091393000 -0.094430000 0.000000000

H 1.091393000 0.094430000 0.000000000

Br -6.820197000 0.037074000 6.847344000

Br -6.820197000 0.037074000 -6.847344000

Br 6.820197000 -0.037074000 -6.847344000

Br 6.820197000 -0.037074000 6.847344000

78

p-III p-4C6H4Br-H2P

N -0.039942000 2.040075000 0.000000000

N 0.000000000 0.000000000 2.103652000

N 0.039942000 -2.040075000 0.000000000

N 0.000000000 0.000000000 -2.103652000

C -0.007080000 2.862847000 1.087025000

C 0.054733000 4.260285000 0.675553000

C -0.007080000 2.862847000 -1.087025000

C 0.054733000 4.260285000 -0.675553000

C -0.001705000 1.130331000 -2.884749000

C -0.004640000 0.683279000 -4.245423000

C 0.001705000 -1.130331000 -2.884749000

C 0.004640000 -0.683279000 -4.245423000

C 0.007080000 -2.862847000 -1.087025000

C -0.054733000 -4.260285000 -0.675553000

C 0.007080000 -2.862847000 1.087025000

C -0.054733000 -4.260285000 0.675553000

C 0.001705000 -1.130331000 2.884749000

C 0.004640000 -0.683279000 4.245423000

C -0.001705000 1.130331000 2.884749000

C -0.004640000 0.683279000 4.245423000

C -0.003475000 2.456843000 2.434882000

C -0.003475000 2.456843000 -2.434882000

C 0.003475000 -2.456843000 -2.434882000

C 0.003475000 -2.456843000 2.434882000

C 0.004641000 3.520542000 3.491196000

C 0.004641000 3.520542000 -3.491196000

C -0.004641000 -3.520542000 -3.491196000

C -0.004641000 -3.520542000 3.491196000

H 0.013007000 -1.333526000 -5.102854000

H -0.013007000 1.333526000 -5.102854000

H 0.107502000 5.110892000 -1.334051000

H 0.107502000 5.110892000 1.334051000

H -0.013007000 1.333526000 5.102854000

H 0.013007000 -1.333526000 5.102854000

H -0.107502000 -5.110892000 1.334051000

H -0.107502000 -5.110892000 -1.334051000

C -1.155894000 4.242145000 3.787084000

C 1.170793000 3.815402000 4.204046000

C -1.158971000 5.231716000 4.766832000

C 1.185372000 4.803750000 5.185112000

H -2.069910000 4.026241000 3.248107000

H -2.064423000 5.779674000 4.988263000

H 2.095725000 5.025914000 5.724593000

H 2.081834000 3.272559000 3.984889000

C 1.170793000 3.815402000 -4.204046000

C -1.155894000 4.242145000 -3.787084000

C 1.185372000 4.803750000 -5.185112000

C -1.158971000 5.231716000 -4.766832000

H 2.081834000 3.272559000 -3.984889000

H 2.095725000 5.025914000 -5.724593000

H -2.064423000 5.779674000 -4.988263000

H -2.069910000 4.026241000 -3.248107000

C -1.170793000 -3.815402000 -4.204046000

C 1.155894000 -4.242145000 -3.787084000

C -1.185372000 -4.803750000 -5.185112000

C 1.158971000 -5.231716000 -4.766832000

H -2.081834000 -3.272559000 -3.984889000

H -2.095725000 -5.025914000 -5.724593000

H 2.064423000 -5.779674000 -4.988263000

H 2.069910000 -4.026241000 -3.248107000

C 1.155894000 -4.242145000 3.787084000

C -1.170793000 -3.815402000 4.204046000

C 1.158971000 -5.231716000 4.766832000

C -1.185372000 -4.803750000 5.185112000

H 2.069910000 -4.026241000 3.248107000

H 2.064423000 -5.779674000 4.988263000

H -2.095725000 -5.025914000 5.724593000

H -2.081834000 -3.272559000 3.984889000

C -0.015931000 -5.503734000 5.458148000

C 0.015931000 5.503734000 5.458148000

C 0.015931000 5.503734000 -5.458148000

C -0.015931000 -5.503734000 -5.458148000

H 0.000000000 0.000000000 -1.092190000

H 0.000000000 0.000000000 1.092190000

Br -0.023676000 -6.862582000 6.805322000

Br 0.023676000 6.862582000 6.805322000

Br 0.023676000 6.862582000 -6.805322000

Br -0.023676000 -6.862582000 -6.805322000

78

p-IV p-4C6H4Br-H2P

N 2.039096000 0.000000000 0.000000000

N 0.000000000 0.000000000 2.102665000

N -2.039096000 0.000000000 0.000000000

N 0.000000000 0.000000000 -2.102665000

C 2.862553000 0.004303000 1.086888000

C 4.261505000 0.000190000 0.675593000

C 2.862553000 -0.004303000 -1.086888000

C 4.261505000 -0.000190000 -0.675593000

C 1.130122000 0.000847000 -2.883835000

C 0.683323000 -0.002087000 -4.244747000

C -1.130122000 -0.000847000 -2.883835000

C -0.683323000 0.002087000 -4.244747000

C -2.862553000 0.004303000 -1.086888000

C -4.261505000 0.000190000 -0.675593000

C -2.862553000 -0.004303000 1.086888000

C -4.261505000 -0.000190000 0.675593000

C -1.130122000 0.000847000 2.883835000

C -0.683323000 -0.002087000 4.244747000

C 1.130122000 -0.000847000 2.883835000

C 0.683323000 0.002087000 4.244747000

C 2.456170000 0.003168000 2.434144000

C 2.456170000 -0.003168000 -2.434144000

C -2.456170000 0.003168000 -2.434144000

C -2.456170000 -0.003168000 2.434144000

C 3.519590000 0.007245000 3.492162000

C 3.519590000 -0.007245000 -3.492162000

C -3.519590000 0.007245000 -3.492162000

C -3.519590000 -0.007245000 3.492162000

H -1.334387000 0.006460000 -5.101740000

H 1.334387000 -0.006460000 -5.101740000

H 5.113328000 0.002582000 -1.334775000

H 5.113328000 -0.002582000 1.334775000

H 1.334387000 0.006460000 5.101740000

H -1.334387000 -0.006460000 5.101740000

H -5.113328000 0.002582000 1.334775000

H -5.113328000 -0.002582000 -1.334775000

C 4.168030000 1.193006000 3.849417000

C 3.884463000 -1.173859000 4.144714000

C 5.156050000 1.205963000 4.830890000

C 4.871379000 -1.178495000 5.127538000

H 3.897350000 2.118415000 3.356459000

H 5.648645000 2.130289000 5.099407000

H 5.147472000 -2.099767000 5.621670000

H 3.396648000 -2.103288000 3.878304000

C 4.168030000 -1.193006000 -3.849417000

C 3.884463000 1.173859000 -4.144714000

C 5.156050000 -1.205963000 -4.830890000

C 4.871379000 1.178495000 -5.127538000

H 3.897350000 -2.118415000 -3.356459000

H 5.648645000 -2.130289000 -5.099407000

H 5.147472000 2.099767000 -5.621670000

H 3.396648000 2.103288000 -3.878304000

C -4.168030000 1.193006000 -3.849417000

C -3.884463000 -1.173859000 -4.144714000

C -5.156050000 1.205963000 -4.830890000

C -4.871379000 -1.178495000 -5.127538000

H -3.897350000 2.118415000 -3.356459000

H -5.648645000 2.130289000 -5.099407000

H -5.147472000 -2.099767000 -5.621670000

H -3.396648000 -2.103288000 -3.878304000

C -4.168030000 -1.193006000 3.849417000

C -3.884463000 1.173859000 4.144714000

C -5.156050000 -1.205963000 4.830890000

C -4.871379000 1.178495000 5.127538000

H -3.897350000 -2.118415000 3.356459000

H -5.648645000 -2.130289000 5.099407000

H -5.147472000 2.099767000 5.621670000

H -3.396648000 2.103288000 3.878304000

C -5.498905000 -0.015819000 5.461971000

C 5.498905000 0.015819000 5.461971000

C 5.498905000 -0.015819000 -5.461971000

C -5.498905000 0.015819000 -5.461971000

H 0.000000000 0.000000000 -1.091214000

H 0.000000000 0.000000000 1.091214000

Br 6.855640000 -0.021688000 -6.811457000

Br -6.855640000 0.021688000 -6.811457000

Br -6.855640000 -0.021688000 6.811457000

Br 6.855640000 0.021688000 6.811457000

78

p-V p-4C6H4Br-H2P

N -2.038206000 0.000000000 0.000000000

N 0.000000000 2.102084000 0.000000000

N 2.038206000 0.000000000 0.000000000

N 0.000000000 -2.102084000 0.000000000

C -2.861770000 1.086677000 0.000000000

C -4.260903000 0.675643000 0.000000000

C -2.861770000 -1.086677000 0.000000000

C -4.260903000 -0.675643000 0.000000000

C -1.129920000 -2.883308000 0.000000000

C -0.683379000 -4.244436000 0.000000000

C 1.129920000 -2.883308000 0.000000000

C 0.683379000 -4.244436000 0.000000000

C 2.861770000 -1.086677000 0.000000000

C 4.260903000 -0.675643000 0.000000000

C 2.861770000 1.086677000 0.000000000

C 4.260903000 0.675643000 0.000000000

C 1.129920000 2.883308000 0.000000000

C 0.683379000 4.244436000 0.000000000

C -1.129920000 2.883308000 0.000000000

C -0.683379000 4.244436000 0.000000000

C -2.455404000 2.433493000 0.000000000

C -2.455404000 -2.433493000 0.000000000

C 2.455404000 -2.433493000 0.000000000

C 2.455404000 2.433493000 0.000000000

C -3.519586000 3.491910000 0.000000000

C -3.519586000 -3.491910000 0.000000000

C 3.519586000 -3.491910000 0.000000000

C 3.519586000 3.491910000 0.000000000

H 1.335272000 -5.100973000 0.000000000

H -1.335272000 -5.100973000 0.000000000

H -5.112180000 -1.335767000 0.000000000

H -5.112180000 1.335767000 0.000000000

H -1.335272000 5.100973000 0.000000000

H 1.335272000 5.100973000 0.000000000

H 5.112180000 1.335767000 0.000000000

H 5.112180000 -1.335767000 0.000000000

C -4.025930000 3.996126000 1.201060000

C -4.025930000 3.996126000 -1.201060000

C -5.013958000 4.977924000 1.209919000

C -5.013958000 4.977924000 -1.209919000

H -3.646253000 3.616300000 2.141465000

H -5.398564000 5.359183000 2.145785000

H -5.398564000 5.359183000 -2.145785000

H -3.646253000 3.616300000 -2.141465000

C -4.025930000 -3.996126000 -1.201060000

C -4.025930000 -3.996126000 1.201060000

C -5.013958000 -4.977924000 -1.209919000

C -5.013958000 -4.977924000 1.209919000

H -3.646253000 -3.616300000 -2.141465000

H -5.398564000 -5.359183000 -2.145785000

H -5.398564000 -5.359183000 2.145785000

H -3.646253000 -3.616300000 2.141465000

C 4.025930000 -3.996126000 1.201060000

C 4.025930000 -3.996126000 -1.201060000

C 5.013958000 -4.977924000 1.209919000

C 5.013958000 -4.977924000 -1.209919000

H 3.646253000 -3.616300000 2.141465000

H 5.398564000 -5.359183000 2.145785000

H 5.398564000 -5.359183000 -2.145785000

H 3.646253000 -3.616300000 -2.141465000

C 4.025930000 3.996126000 -1.201060000

C 4.025930000 3.996126000 1.201060000

C 5.013958000 4.977924000 -1.209919000

C 5.013958000 4.977924000 1.209919000

H 3.646253000 3.616300000 -2.141465000

H 5.398564000 5.359183000 -2.145785000

H 5.398564000 5.359183000 2.145785000

H 3.646253000 3.616300000 2.141465000

C 5.499244000 5.460311000 0.000000000

C -5.499244000 5.460311000 0.000000000

C -5.499244000 -5.460311000 0.000000000

C 5.499244000 -5.460311000 0.000000000

H 0.000000000 -1.090651000 0.000000000

H 0.000000000 1.090651000 0.000000000

Br -6.856677000 -6.809259000 0.000000000

Br 6.856677000 -6.809259000 0.000000000

Br 6.856677000 6.809259000 0.000000000

Br -6.856677000 6.809259000 0.000000000

78

p-VI p-4C6H4Br-H2P

N 0.000000000 2.091454000 0.000000000

N 0.000000000 0.000000000 2.117416000

N 0.000000000 -2.091454000 0.000000000

N 0.000000000 0.000000000 -2.117416000

C 0.000000000 2.914590000 1.123433000

C 0.000000000 4.280437000 0.662970000

C 0.000000000 2.914590000 -1.123433000

C 0.000000000 4.280437000 -0.662970000

C 0.000000000 1.168647000 -2.903980000

C 0.000000000 0.670177000 -4.228233000

C 0.000000000 -1.168647000 -2.903980000

C 0.000000000 -0.670177000 -4.228233000

C 0.000000000 -2.914590000 -1.123433000

C 0.000000000 -4.280437000 -0.662970000

C 0.000000000 -2.914590000 1.123433000

C 0.000000000 -4.280437000 0.662970000

C 0.000000000 -1.168647000 2.903980000

C 0.000000000 -0.670177000 4.228233000

C 0.000000000 1.168647000 2.903980000

C 0.000000000 0.670177000 4.228233000

C 0.000000000 2.553407000 2.520254000

C 0.000000000 2.553407000 -2.520254000

C 0.000000000 -2.553407000 -2.520254000

C 0.000000000 -2.553407000 2.520254000

C 0.000000000 3.670869000 3.653962000

C 0.000000000 3.670869000 -3.653962000

C 0.000000000 -3.670869000 -3.653962000

C 0.000000000 -3.670869000 3.653962000

H 0.000000000 -1.161720000 -5.159217000

H 0.000000000 1.161720000 -5.159217000

H 0.000000000 5.212382000 -1.156343000

H 0.000000000 5.212382000 1.156343000

H 0.000000000 1.161720000 5.159217000

H 0.000000000 -1.161720000 5.159217000

H 0.000000000 -5.212382000 1.156343000

H 0.000000000 -5.212382000 -1.156343000

C 0.000000000 3.437405000 5.056514000

C 0.000000000 5.075152000 3.435918000

C 0.000000000 4.400331000 6.061592000

C 0.000000000 6.070039000 4.408799000

H 0.000000000 2.476069000 5.489424000

H 0.000000000 4.069289000 7.091225000

H 0.000000000 7.102933000 4.088100000

H 0.000000000 5.512539000 2.477035000

C 0.000000000 3.437405000 -5.056514000

C 0.000000000 5.075152000 -3.435918000

C 0.000000000 4.400331000 -6.061592000

C 0.000000000 6.070039000 -4.408799000

H 0.000000000 2.476069000 -5.489424000

H 0.000000000 4.069289000 -7.091225000

H 0.000000000 7.102933000 -4.088100000

H 0.000000000 5.512539000 -2.477035000

C 0.000000000 -5.075152000 -3.435918000

C 0.000000000 -3.437405000 -5.056514000

C 0.000000000 -6.070039000 -4.408799000

C 0.000000000 -4.400331000 -6.061592000

H 0.000000000 -5.512539000 -2.477035000

H 0.000000000 -7.102933000 -4.088100000

H 0.000000000 -4.069289000 -7.091225000

H 0.000000000 -2.476069000 -5.489424000

C 0.000000000 -3.437405000 5.056514000

C 0.000000000 -5.075152000 3.435918000

C 0.000000000 -4.400331000 6.061592000

C 0.000000000 -6.070039000 4.408799000

H 0.000000000 -2.476069000 5.489424000

H 0.000000000 -4.069289000 7.091225000

H 0.000000000 -7.102933000 4.088100000

H 0.000000000 -5.512539000 2.477035000

C 0.000000000 -5.743404000 5.748752000

C 0.000000000 5.743404000 5.748752000

C 0.000000000 5.743404000 -5.748752000

C 0.000000000 -5.743404000 -5.748752000

H 0.000000000 0.000000000 -1.105826000

H 0.000000000 0.000000000 1.105826000

Br 0.000000000 -7.081892000 7.101706000

Br 0.000000000 7.081892000 7.101706000

Br 0.000000000 7.081892000 -7.101706000

Br 0.000000000 -7.081892000 -7.101706000

78

m-I(I) m-4C6H4Br-H2P

N -0.593366000 -1.952236000 -0.002969000

N 2.012836000 -0.613447000 -0.032854000

N 0.593366000 1.952236000 -0.002969000

N -2.012836000 0.613447000 -0.032854000

C 0.206754000 -3.055623000 -0.040930000

C -0.593366000 -4.271412000 -0.128428000

C -1.872639000 -2.422268000 -0.045296000

C -1.885793000 -3.877774000 -0.131343000

C -3.087870000 -0.241171000 0.003850000

C -4.257954000 0.581198000 0.079338000

C -2.430830000 1.921536000 0.008328000

C -3.860779000 1.888708000 0.082585000

C -0.206754000 3.055623000 -0.040930000

C 0.593366000 4.271412000 -0.128428000

C 1.872639000 2.422268000 -0.045296000

C 1.885793000 3.877774000 -0.131343000

C 3.087870000 0.241171000 0.003850000

C 4.257954000 -0.581198000 0.079338000

C 2.430830000 -1.921536000 0.008328000

C 3.860779000 -1.888708000 0.082585000

C 1.614145000 -3.059385000 -0.011565000

C -3.043162000 -1.640934000 -0.020028000

C -1.614145000 3.059385000 -0.011565000

C 3.043162000 1.640934000 -0.020028000

C 2.314551000 -4.384761000 0.004138000

C -4.364227000 -2.350046000 -0.017519000

C -2.314551000 4.384761000 0.004138000

C 4.364227000 2.350046000 -0.017519000

H -4.490862000 2.759189000 0.140183000

H -5.265661000 0.207584000 0.134135000

H -2.762922000 -4.499096000 -0.198459000

H -0.210975000 -5.276114000 -0.193274000

H 4.490862000 -2.759189000 0.140183000

H 5.265661000 -0.207584000 0.134135000

H 2.762922000 4.499096000 -0.198459000

H 0.210975000 5.276114000 -0.193274000

C 2.971105000 -4.848721000 -1.141366000

C 2.324332000 -5.174353000 1.158248000

C 3.617585000 -6.079047000 -1.114725000

C 2.978361000 -6.402764000 1.167671000

H 2.983491000 -7.004721000 2.067837000

H 1.821821000 -4.819926000 2.048900000

C -5.162734000 -2.382841000 -1.164905000

C -4.815385000 -2.990094000 1.142348000

C -6.386409000 -3.046055000 -1.154945000

C -6.041229000 -3.645311000 1.135258000

H -4.817286000 -1.895220000 -2.067410000

H -6.994217000 -3.071392000 -2.050839000

C -2.971105000 4.848721000 -1.141366000

C -2.324332000 5.174353000 1.158248000

C -3.617585000 6.079047000 -1.114725000

C -2.978361000 6.402764000 1.167671000

H -2.983491000 7.004721000 2.067837000

H -1.821821000 4.819926000 2.048900000

C 5.162734000 2.382841000 -1.164905000

C 4.815385000 2.990094000 1.142348000

C 6.386409000 3.046055000 -1.154945000

C 6.041229000 3.645311000 1.135258000

H 4.817286000 1.895220000 -2.067410000

H 6.994217000 3.071392000 -2.050839000

C 6.838483000 3.684318000 -0.002797000

C 3.632178000 -6.868078000 0.029446000

C -6.838483000 -3.684318000 -0.002797000

C -3.632178000 6.868078000 0.029446000

H -1.045076000 0.319887000 -0.050728000

H 1.045076000 -0.319887000 -0.050728000

H -4.140693000 7.822036000 0.032718000

H -7.788331000 -4.200342000 0.009148000

H 4.140693000 -7.822036000 0.032718000

H 7.788331000 4.200342000 0.009148000

Br 6.644616000 4.511613000 2.733051000

Br -4.505018000 6.700147000 -2.694206000

Br -6.644616000 -4.511613000 2.733051000

Br 4.505018000 -6.700147000 -2.694206000

H 2.966741000 -4.254430000 -2.044638000

H 4.212211000 2.969933000 2.039417000

H -2.966741000 4.254430000 -2.044638000

H -4.212211000 -2.969933000 2.039417000

78

m-I(II) m-4C6H4Br-H2P

N 0.000000000 2.038728000 0.000000000

N 0.000000000 0.000000000 -2.102776000

N 0.000000000 -2.038728000 0.000000000

N 0.000000000 0.000000000 2.102776000

C -0.005772000 2.862268000 -1.086619000

C -0.001757000 4.261338000 -0.675554000

C 0.005772000 2.862268000 1.086619000

C 0.001757000 4.261338000 0.675554000

C 0.001035000 1.129853000 2.884031000

C 0.002892000 0.683267000 4.245085000

C -0.001035000 -1.129853000 2.884031000

C -0.002892000 -0.683267000 4.245085000

C -0.005772000 -2.862268000 1.086619000

C -0.001757000 -4.261338000 0.675554000

C 0.005772000 -2.862268000 -1.086619000

C 0.001757000 -4.261338000 -0.675554000

C 0.001035000 -1.129853000 -2.884031000

C 0.002892000 -0.683267000 -4.245085000

C -0.001035000 1.129853000 -2.884031000

C -0.002892000 0.683267000 -4.245085000

C -0.006443000 2.455194000 -2.433355000

C 0.006443000 2.455194000 2.433355000

C -0.006443000 -2.455194000 2.433355000

C 0.006443000 -2.455194000 -2.433355000

C -0.016058000 3.519700000 -3.491317000

C 0.016058000 3.519700000 3.491317000

C -0.016058000 -3.519700000 3.491317000

C 0.016058000 -3.519700000 -3.491317000

H -0.007115000 -1.334272000 5.102148000

H 0.007115000 1.334272000 5.102148000

H 0.001093000 5.112919000 1.335101000

H -0.001093000 5.112919000 -1.335101000

H -0.007115000 1.334272000 -5.102148000

H 0.007115000 -1.334272000 -5.102148000

H 0.001093000 -5.112919000 -1.335101000

H -0.001093000 -5.112919000 1.335101000

C 1.176138000 3.898803000 -4.117239000

C -1.209265000 4.143956000 -3.865970000

C 1.156144000 4.885951000 -5.096127000

C -1.210934000 5.130235000 -4.848257000

H -2.140426000 5.607377000 -5.132983000

H -2.134983000 3.853330000 -3.386151000

C 1.209265000 4.143956000 3.865970000

C -1.176138000 3.898803000 4.117239000

C 1.210934000 5.130235000 4.848257000

C -1.156144000 4.885951000 5.096127000

H 2.134983000 3.853330000 3.386151000

H 2.140426000 5.607377000 5.132983000

C 1.176138000 -3.898803000 4.117239000

C -1.209265000 -4.143956000 3.865970000

C 1.156144000 -4.885951000 5.096127000

C -1.210934000 -5.130235000 4.848257000

H -2.140426000 -5.607377000 5.132983000

H -2.134983000 -3.853330000 3.386151000

C 1.209265000 -4.143956000 -3.865970000

C -1.176138000 -3.898803000 -4.117239000

C 1.210934000 -5.130235000 -4.848257000

C -1.156144000 -4.885951000 -5.096127000

H 2.134983000 -3.853330000 -3.386151000

H 2.140426000 -5.607377000 -5.132983000

C 0.026400000 -5.511235000 -5.473658000

C -0.026400000 5.511235000 -5.473658000

C 0.026400000 5.511235000 5.473658000

C -0.026400000 -5.511235000 5.473658000

H 0.000000000 0.000000000 1.091322000

H 0.000000000 0.000000000 -1.091322000

H -0.023592000 -6.276887000 6.236841000

H 0.023592000 6.276887000 6.236841000

H -0.023592000 6.276887000 -6.236841000

H 0.023592000 -6.276887000 -6.236841000

Br -2.797947000 -5.395495000 -5.940286000

Br 2.797947000 -5.395495000 5.940286000

Br -2.797947000 5.395495000 5.940286000

Br 2.797947000 5.395495000 -5.940286000

H 2.107905000 3.428152000 -3.835197000

H -2.107905000 -3.428152000 -3.835197000

H 2.107905000 -3.428152000 3.835197000

H -2.107905000 3.428152000 3.835197000

78

m-II m-4C6H4Br-H2P

N 0.421604000 -1.950476000 -0.116986000

N -1.933857000 -0.283101000 -0.624685000

N -0.156724000 2.048565000 -0.685260000

N 2.189982000 0.388479000 -0.117766000

C -0.531556000 -2.925244000 -0.096460000

C 0.057923000 -4.217600000 0.232929000

C 1.597600000 -2.578103000 0.170162000

C 1.381253000 -4.001802000 0.398751000

C 3.119564000 -0.599609000 0.098815000

C 4.398054000 0.045100000 0.128761000

C 2.800145000 1.615158000 -0.219810000

C 4.205082000 1.384051000 -0.064514000

C 0.785645000 3.032468000 -0.629456000

C 0.171489000 4.345651000 -0.785074000

C -1.344767000 2.686302000 -0.887877000

C -1.152707000 4.130521000 -0.945405000

C -2.853474000 0.696343000 -0.911879000

C -4.111070000 0.033677000 -1.087050000

C -2.532486000 -1.519479000 -0.601693000

C -3.916941000 -1.305911000 -0.899953000

C -1.905652000 -2.745319000 -0.343818000

C 2.863369000 -1.968031000 0.252095000

C 2.167777000 2.845618000 -0.438778000

C -2.603680000 2.070383000 -1.019519000

C -2.786563000 -3.958333000 -0.338674000

C 4.050717000 -2.841657000 0.526461000

C 3.053233000 4.054900000 -0.473300000

C -3.788396000 2.944084000 -1.303927000

H 4.959754000 2.150072000 -0.106402000

H 5.336061000 -0.462989000 0.270474000

H 2.137700000 -4.721779000 0.662057000

H -0.475435000 -5.147589000 0.335354000

H -4.655884000 -2.085258000 -0.967812000

H -5.034694000 0.528291000 -1.332659000

H -1.928633000 4.866281000 -1.073770000

H 0.686450000 5.291141000 -0.757070000

C -3.659882000 -4.190933000 0.729825000

C -2.750635000 -4.871993000 -1.396756000

C -4.471870000 -5.319248000 0.723479000

C -3.572131000 -5.995325000 -1.387597000

H -3.539558000 -6.694727000 -2.213716000

H -2.080196000 -4.696374000 -2.228072000

C 4.660335000 -2.848518000 1.784804000

C 4.565223000 -3.664225000 -0.482027000

C 5.760275000 -3.664818000 2.032083000

C 5.666020000 -4.470958000 -0.218370000

H 4.263855000 -2.219405000 2.571348000

H 6.221045000 -3.667884000 3.012070000

C 3.599107000 4.563003000 0.710878000

C 3.347845000 4.690605000 -1.683489000

C 4.419439000 5.684388000 0.666327000

C 4.172718000 5.811218000 -1.709807000

H 4.398222000 6.293662000 -2.652733000

H 2.932225000 4.300502000 -2.603548000

C -3.975667000 3.504161000 -2.571494000

C -4.725818000 3.209221000 -0.299274000

C -5.078665000 4.312472000 -2.830167000

C -5.820543000 4.020611000 -0.574534000

H -3.256571000 3.299897000 -3.354199000

H -5.216872000 4.737982000 -3.816354000

C -6.013102000 4.579330000 -1.832621000

C -4.441883000 -6.230511000 -0.325654000

C 6.274909000 -4.484884000 1.031160000

C 4.717215000 6.320089000 -0.533329000

H 1.196417000 0.230583000 -0.222400000

H -0.945320000 -0.120864000 -0.485031000

H 5.357901000 7.190663000 -0.549651000

H 7.129117000 -5.120219000 1.219101000

H -5.080967000 -7.102338000 -0.314611000

H -6.870778000 5.207247000 -2.029493000

Br -7.089140000 4.377584000 0.814733000

Br 5.152198000 6.368796000 2.297980000

Br 6.359482000 -5.586710000 -1.611941000

Br -5.655733000 -5.624098000 2.197576000

H -3.694883000 -3.498650000 1.559666000

H -4.592396000 2.790137000 0.688498000

H 3.375244000 4.088296000 1.656208000

H 4.108224000 -3.667106000 -1.461885000

78

m-III m-4C6H4Br-H2P

N 0.000000000 0.000000000 2.040061000

N -0.474103000 2.049812000 0.000000000

N 0.000000000 0.000000000 -2.040061000

N 0.474103000 -2.049812000 0.000000000

C -0.270619000 1.052589000 2.863441000

C -0.165554000 0.654923000 4.262348000

C 0.270619000 -1.052589000 2.863441000

C 0.165554000 -0.654923000 4.262348000

C 0.702440000 -2.797151000 1.129976000

C 1.093503000 -4.100591000 0.683203000

C 0.702440000 -2.797151000 -1.129976000

C 1.093503000 -4.100591000 -0.683203000

C 0.270619000 -1.052589000 -2.863441000

C 0.165554000 -0.654923000 -4.262348000

C -0.270619000 1.052589000 -2.863441000

C -0.165554000 0.654923000 -4.262348000

C -0.702440000 2.797151000 -1.129976000

C -1.093503000 4.100591000 -0.683203000

C -0.702440000 2.797151000 1.129976000

C -1.093503000 4.100591000 0.683203000

C -0.601749000 2.358312000 2.456015000

C 0.601749000 -2.358312000 2.456015000

C 0.601749000 -2.358312000 -2.456015000

C -0.601749000 2.358312000 -2.456015000

C -0.886536000 3.377611000 3.518892000

C 0.886536000 -3.377611000 3.518892000

C 0.886536000 -3.377611000 -3.518892000

C -0.886536000 3.377611000 -3.518892000

H 1.350724000 -4.918547000 -1.333560000

H 1.350724000 -4.918547000 1.333560000

H 0.322525000 -1.294597000 5.114453000

H -0.322525000 1.294597000 5.114453000

H -1.350724000 4.918547000 1.333560000

H -1.350724000 4.918547000 -1.333560000

H -0.322525000 1.294597000 -5.114453000

H 0.322525000 -1.294597000 -5.114453000

C 0.068982000 4.349927000 3.833945000

C -2.104119000 3.374232000 4.206210000

C -0.204473000 5.290706000 4.820317000

C -2.361638000 4.324535000 5.189942000

H -3.308940000 4.315538000 5.714587000

H -2.848925000 2.626906000 3.964750000

C 2.104119000 -3.374232000 4.206210000

C -0.068982000 -4.349927000 3.833945000

C 2.361638000 -4.324535000 5.189942000

C 0.204473000 -5.290706000 4.820317000

H 2.848925000 -2.626906000 3.964750000

H 3.308940000 -4.315538000 5.714587000

C -0.068982000 -4.349927000 -3.833945000

C 2.104119000 -3.374232000 -4.206210000

C 0.204473000 -5.290706000 -4.820317000

C 2.361638000 -4.324535000 -5.189942000

H 3.308940000 -4.315538000 -5.714587000

H 2.848925000 -2.626906000 -3.964750000

C -2.104119000 3.374232000 -4.206210000

C 0.068982000 4.349927000 -3.833945000

C -2.361638000 4.324535000 -5.189942000

C -0.204473000 5.290706000 -4.820317000

H -2.848925000 2.626906000 -3.964750000

H -3.308940000 4.315538000 -5.714587000

C -1.412754000 5.293298000 -5.507275000

C -1.412754000 5.293298000 5.507275000

C 1.412754000 -5.293298000 5.507275000

C 1.412754000 -5.293298000 -5.507275000

H 0.196997000 -1.076958000 0.000000000

H -0.196997000 1.076958000 0.000000000

H 1.609012000 -6.032793000 -6.271012000

H 1.609012000 -6.032793000 6.271012000

H -1.609012000 6.032793000 6.271012000

H -1.609012000 6.032793000 -6.271012000

Br 1.117564000 6.610502000 -5.241931000

Br -1.117564000 -6.610502000 -5.241931000

Br -1.117564000 -6.610502000 5.241931000

Br 1.117564000 6.610502000 5.241931000

H 1.017830000 4.362885000 3.315590000

H 1.017830000 4.362885000 -3.315590000

H -1.017830000 -4.362885000 -3.315590000

H -1.017830000 -4.362885000 3.315590000

78

m-IV m-4C6H4Br-H2P

N -1.962263000 0.557173000 0.000000000

N 0.000000000 0.000000000 2.103634000

N 1.962263000 -0.557173000 0.000000000

N 0.000000000 0.000000000 -2.103634000

C -2.765065000 0.740698000 1.086771000

C -4.130082000 1.046950000 0.675523000

C -2.765065000 0.740698000 -1.086771000

C -4.130082000 1.046950000 -0.675523000

C -1.091902000 0.291089000 -2.884833000

C -0.659379000 0.178945000 -4.245719000

C 1.091902000 -0.291089000 -2.884833000

C 0.659379000 -0.178945000 -4.245719000

C 2.765065000 -0.740698000 -1.086771000

C 4.130082000 -1.046950000 -0.675523000

C 2.765065000 -0.740698000 1.086771000

C 4.130082000 -1.046950000 0.675523000

C 1.091902000 -0.291089000 2.884833000

C 0.659379000 -0.178945000 4.245719000

C -1.091902000 0.291089000 2.884833000

C -0.659379000 0.178945000 4.245719000

C -2.372675000 0.633445000 2.434017000

C -2.372675000 0.633445000 -2.434017000

C 2.372675000 -0.633445000 -2.434017000

C 2.372675000 -0.633445000 2.434017000

C -3.402651000 0.903031000 3.490687000

C -3.402651000 0.903031000 -3.490687000

C 3.402651000 -0.903031000 -3.490687000

C 3.402651000 -0.903031000 3.490687000

H 1.286174000 -0.351881000 -5.103268000

H -1.286174000 0.351881000 -5.103268000

H -4.964238000 1.220127000 -1.334477000

H -4.964238000 1.220127000 1.334477000

H -1.286174000 0.351881000 5.103268000

H 1.286174000 -0.351881000 5.103268000

H 4.964238000 -1.220127000 1.334477000

H 4.964238000 -1.220127000 -1.334477000

C -4.004154000 -0.158843000 4.174995000

C -3.775033000 2.212897000 3.807195000

C -4.957253000 0.103251000 5.152585000

C -4.730316000 2.457045000 4.789584000

H -5.009838000 3.475299000 5.029852000

H -3.311111000 3.038709000 3.283400000

C -3.775033000 2.212897000 -3.807195000

C -4.004154000 -0.158843000 -4.174995000

C -4.730316000 2.457045000 -4.789584000

C -4.957253000 0.103251000 -5.152585000

H -3.311111000 3.038709000 -3.283400000

H -5.009838000 3.475299000 -5.029852000

C 4.004154000 0.158843000 -4.174995000

C 3.775033000 -2.212897000 -3.807195000

C 4.957253000 -0.103251000 -5.152585000

C 4.730316000 -2.457045000 -4.789584000

H 5.009838000 -3.475299000 -5.029852000

H 3.311111000 -3.038709000 -3.283400000

C 3.775033000 -2.212897000 3.807195000

C 4.004154000 0.158843000 4.174995000

C 4.730316000 -2.457045000 4.789584000

C 4.957253000 -0.103251000 5.152585000

H 3.311111000 -3.038709000 3.283400000

H 5.009838000 -3.475299000 5.029852000

C 5.331648000 -1.402978000 5.472778000

C -5.331648000 1.402978000 5.472778000

C -5.331648000 1.402978000 -5.472778000

C 5.331648000 -1.402978000 -5.472778000

H 0.000000000 0.000000000 -1.092177000

H 0.000000000 0.000000000 1.092177000

H 6.074184000 -1.588535000 -6.236232000

H -6.074184000 1.588535000 -6.236232000

H -6.074184000 1.588535000 6.236232000

H 6.074184000 -1.588535000 6.236232000

Br 5.773618000 1.362634000 6.075656000

Br 5.773618000 1.362634000 -6.075656000

Br -5.773618000 -1.362634000 -6.075656000

Br -5.773618000 -1.362634000 6.075656000

H -3.732072000 -1.178035000 3.937495000

H 3.732072000 1.178035000 3.937495000

H 3.732072000 1.178035000 -3.937495000

H -3.732072000 -1.178035000 -3.937495000

78

m-V m-4C6H4Br-H2P

N -2.040199000 0.000000000 -0.817672000

N 0.000000000 2.104590000 -0.786360000

N 2.040199000 0.000000000 -0.817672000

N 0.000000000 -2.104590000 -0.786360000

C -2.862445000 1.086888000 -0.774643000

C -4.258275000 0.675538000 -0.683168000

C -2.862445000 -1.086888000 -0.774643000

C -4.258275000 -0.675538000 -0.683168000

C -1.130166000 -2.884818000 -0.824579000

C -0.683229000 -4.243508000 -0.898635000

C 1.130166000 -2.884818000 -0.824579000

C 0.683229000 -4.243508000 -0.898635000

C 2.862445000 -1.086888000 -0.774643000

C 4.258275000 -0.675538000 -0.683168000

C 2.862445000 1.086888000 -0.774643000

C 4.258275000 0.675538000 -0.683168000

C 1.130166000 2.884818000 -0.824579000

C 0.683229000 4.243508000 -0.898635000

C -1.130166000 2.884818000 -0.824579000

C -0.683229000 4.243508000 -0.898635000

C -2.456334000 2.434458000 -0.802420000

C -2.456334000 -2.434458000 -0.802420000

C 2.456334000 -2.434458000 -0.802420000

C 2.456334000 2.434458000 -0.802420000

C -3.520578000 3.490320000 -0.813101000

C -3.520578000 -3.490320000 -0.813101000

C 3.520578000 -3.490320000 -0.813101000

C 3.520578000 3.490320000 -0.813101000

H 1.332936000 -5.099642000 -0.952837000

H -1.332936000 -5.099642000 -0.952837000

H -5.107539000 -1.334018000 -0.612228000

H -5.107539000 1.334018000 -0.612228000

H -1.332936000 5.099642000 -0.952837000

H 1.332936000 5.099642000 -0.952837000

H 5.107539000 1.334018000 -0.612228000

H 5.107539000 -1.334018000 -0.612228000

C -3.771063000 4.250324000 0.334984000

C -4.275551000 3.732492000 -1.965021000

C -4.760258000 5.226824000 0.313168000

C -5.260537000 4.715661000 -1.969794000

H -3.201744000 4.070907000 1.236545000

H -5.836771000 4.898356000 -2.868298000

H -4.084357000 3.150965000 -2.857605000

C -4.275551000 -3.732492000 -1.965021000

C -3.771063000 -4.250324000 0.334984000

C -5.260537000 -4.715661000 -1.969794000

C -4.760258000 -5.226824000 0.313168000

H -4.084357000 -3.150965000 -2.857605000

H -5.836771000 -4.898356000 -2.868298000

H -3.201744000 -4.070907000 1.236545000

C 3.771063000 -4.250324000 0.334984000

C 4.275551000 -3.732492000 -1.965021000

C 4.760258000 -5.226824000 0.313168000

C 5.260537000 -4.715661000 -1.969794000

H 3.201744000 -4.070907000 1.236545000

H 5.836771000 -4.898356000 -2.868298000

H 4.084357000 -3.150965000 -2.857605000

C 4.275551000 3.732492000 -1.965021000

C 3.771063000 4.250324000 0.334984000

C 5.260537000 4.715661000 -1.969794000

C 4.760258000 5.226824000 0.313168000

H 4.084357000 3.150965000 -2.857605000

H 5.836771000 4.898356000 -2.868298000

H 3.201744000 4.070907000 1.236545000

C 5.513170000 5.473362000 -0.828939000

C -5.513170000 5.473362000 -0.828939000

C -5.513170000 -5.473362000 -0.828939000

C 5.513170000 -5.473362000 -0.828939000

H 0.000000000 -1.093300000 -0.768060000

H 0.000000000 1.093300000 -0.768060000

H 6.277911000 -6.237448000 -0.828496000

H -6.277911000 -6.237448000 -0.828496000

H -6.277911000 6.237448000 -0.828496000

H 6.277911000 6.237448000 -0.828496000

Br -5.093255000 6.252004000 1.895827000

Br 5.093255000 6.252004000 1.895827000

Br 5.093255000 -6.252004000 1.895827000

Br -5.093255000 -6.252004000 1.895827000

78

o-I o-4C6H4Br-H2P

N 2.037933000 0.000000000 0.000000000

N 0.000000000 0.000000000 2.101725000

N -2.037933000 0.000000000 0.000000000

N 0.000000000 0.000000000 -2.101725000

C 2.861208000 0.011966000 1.085873000

C 4.260383000 0.007740000 0.675334000

C 2.861208000 -0.011966000 -1.085873000

C 4.260383000 -0.007740000 -0.675334000

C 1.128964000 -0.011240000 -2.882775000

C 0.683110000 -0.006327000 -4.243738000

C -1.128964000 0.011240000 -2.882775000

C -0.683110000 0.006327000 -4.243738000

C -2.861208000 0.011966000 -1.085873000

C -4.260383000 0.007740000 -0.675334000

C -2.861208000 -0.011966000 1.085873000

C -4.260383000 -0.007740000 0.675334000

C -1.128964000 -0.011240000 2.882775000

C -0.683110000 -0.006327000 4.243738000

C 1.128964000 0.011240000 2.882775000

C 0.683110000 0.006327000 4.243738000

C 2.452923000 0.024713000 2.431180000

C 2.452923000 -0.024713000 -2.431180000

C -2.452923000 0.024713000 -2.431180000

C -2.452923000 -0.024713000 2.431180000

C 3.516859000 0.013970000 3.488539000

C 3.516859000 -0.013970000 -3.488539000

C -3.516859000 0.013970000 -3.488539000

C -3.516859000 -0.013970000 3.488539000

H -1.334889000 0.013504000 -5.100425000

H 1.334889000 -0.013504000 -5.100425000

H 5.111900000 -0.016236000 -1.335284000

H 5.111900000 0.016236000 1.335284000

H 1.334889000 0.013504000 5.100425000

H -1.334889000 -0.013504000 5.100425000

H -5.111900000 -0.016236000 1.335284000

H -5.111900000 0.016236000 -1.335284000

C 4.057093000 1.178538000 4.045926000

C 4.008754000 -1.211779000 3.956932000

C 5.045869000 1.130200000 5.025999000

C 4.995096000 -1.276503000 4.934427000

H 5.355182000 -2.239114000 5.274432000

H 3.602124000 -2.122649000 3.535640000

C 4.008754000 1.211779000 -3.956932000

C 4.057093000 -1.178538000 -4.045926000

C 4.995096000 1.276503000 -4.934427000

C 5.045869000 -1.130200000 -5.025999000

H 3.602124000 2.122649000 -3.535640000

H 5.355182000 2.239114000 -5.274432000

C -4.057093000 1.178538000 -4.045926000

C -4.008754000 -1.211779000 -3.956932000

C -5.045869000 1.130200000 -5.025999000

C -4.995096000 -1.276503000 -4.934427000

H -5.355182000 -2.239114000 -5.274432000

H -3.602124000 -2.122649000 -3.535640000

C -4.008754000 1.211779000 3.956932000

C -4.057093000 -1.178538000 4.045926000

C -4.995096000 1.276503000 4.934427000

C -5.045869000 -1.130200000 5.025999000

H -3.602124000 2.122649000 3.535640000

H -5.355182000 2.239114000 5.274432000

C -5.514807000 0.101420000 5.470032000

C 5.514807000 -0.101420000 5.470032000

C 5.514807000 0.101420000 -5.470032000

C -5.514807000 -0.101420000 -5.470032000

H 0.000000000 0.000000000 -1.090292000

H 0.000000000 0.000000000 1.090292000

H -6.283744000 -0.137370000 -6.231552000

H 6.283744000 0.137370000 -6.231552000

H 6.283744000 -0.137370000 6.231552000

H -6.283744000 0.137370000 6.231552000

H -5.442267000 -2.049585000 5.434130000

H -5.442267000 2.049585000 -5.434130000

H 5.442267000 -2.049585000 -5.434130000

H 5.442267000 2.049585000 5.434130000

Br 3.454322000 2.904584000 3.474435000

Br -3.454322000 -2.904584000 3.474435000

Br -3.454322000 2.904584000 -3.474435000

Br 3.454322000 -2.904584000 -3.474435000

78

o-II o-4C6H4Br-H2P

N -1.549710000 1.379816000 -0.144054000

N 1.327281000 1.532709000 -0.666633000

N 1.391463000 -1.394161000 -0.664462000

N -1.485030000 -1.546871000 -0.140013000

C -1.415810000 2.735778000 -0.167672000

C -2.699314000 3.387228000 0.065969000

C -2.870572000 1.144501000 0.094420000

C -3.604101000 2.397556000 0.228710000

C -2.822810000 -1.350942000 0.098055000

C -3.409983000 -2.651534000 0.219562000

C -1.190786000 -2.887403000 -0.175190000

C -2.422727000 -3.581189000 0.053080000

C 1.261271000 -2.749925000 -0.620644000

C 2.545827000 -3.401370000 -0.848300000

C 2.710985000 -1.158829000 -0.910911000

C 3.447275000 -2.411854000 -1.029618000

C 2.660445000 1.336541000 -0.929207000

C 3.244135000 2.636900000 -1.068090000

C 1.033336000 2.873221000 -0.628980000

C 2.259743000 3.566718000 -0.885798000

C -0.221170000 3.443589000 -0.387912000

C -3.477642000 -0.119142000 0.201671000

C 0.068614000 -3.457587000 -0.388941000

C 3.314944000 0.104665000 -1.035731000

C -0.286062000 4.942130000 -0.406420000

C -4.948808000 -0.169660000 0.489894000

C 0.127066000 -4.956485000 -0.400590000

C 4.782812000 0.154803000 -1.340858000

H -2.523866000 -4.652398000 0.085846000

H -4.453569000 -2.835729000 0.408761000

H -4.660119000 2.493559000 0.419314000

H -2.870722000 4.450315000 0.099895000

H 2.360318000 4.637911000 -0.920932000

H 4.284010000 2.820902000 -1.276907000

H 4.503642000 -2.507796000 -1.218295000

H 2.721208000 -4.464297000 -0.860368000

C -0.076774000 5.733253000 0.729067000

C -0.568975000 5.603826000 -1.608861000

C -0.146096000 7.123572000 0.674578000

C -0.641453000 6.990329000 -1.679143000

H -0.863266000 7.471844000 -2.623000000

H -0.735507000 5.006416000 -2.496516000

C -5.389179000 -0.172270000 1.820274000

C -5.926318000 -0.215660000 -0.510615000

C -6.741066000 -0.216731000 2.141163000

C -7.284720000 -0.260481000 -0.205263000

H -4.645940000 -0.136158000 2.606909000

H -7.049371000 -0.216239000 3.178865000

C 0.353122000 -5.724710000 0.747366000

C -0.051912000 -5.642516000 -1.609332000

C 0.402130000 -7.116089000 0.698199000

C -0.006054000 -7.030417000 -1.674366000

H -0.147239000 -7.531018000 -2.623782000

H -0.227811000 -5.063156000 -2.507090000

C 5.208388000 0.138228000 -2.675891000

C 5.770926000 0.218891000 -0.351549000

C 6.556432000 0.182211000 -3.012703000

C 7.125688000 0.263250000 -0.673389000

H 4.456596000 0.087756000 -3.453616000

H 6.853351000 0.166927000 -4.053641000

C 7.517458000 0.244939000 -2.007557000

C -0.429086000 7.751833000 -0.533349000

C -7.691132000 -0.260906000 1.124701000

C 0.221948000 -7.768748000 -0.516486000

H -0.809307000 -0.805631000 -0.270300000

H 0.655580000 0.791690000 -0.515978000

H 0.260722000 -8.850252000 -0.552836000

H -8.747372000 -0.295274000 1.360591000

H -0.483065000 8.832543000 -0.573728000

H 8.570926000 0.279089000 -2.255593000

H 7.863037000 0.310683000 0.115941000

H 0.580433000 -7.678822000 1.604021000

H -8.013371000 -0.293883000 -1.003337000

H 0.019551000 7.704417000 1.571325000

Br 0.311991000 4.926920000 2.421916000

Br 5.294930000 0.242747000 1.502749000

Br 0.610802000 -4.884542000 2.448744000

Br -5.429919000 -0.214866000 -2.360822000

78

o-III o-4C6H4Br-H2P

N 0.000000000 0.000000000 2.038183000

N -0.509165000 2.039229000 0.000000000

N 0.000000000 0.000000000 -2.038183000

N 0.509165000 -2.039229000 0.000000000

C -0.266785000 1.052683000 2.861445000

C -0.166089000 0.654640000 4.260631000

C 0.266785000 -1.052683000 2.861445000

C 0.166089000 -0.654640000 4.260631000

C 0.716600000 -2.792257000 1.129038000

C 1.078373000 -4.104235000 0.683145000

C 0.716600000 -2.792257000 -1.129038000

C 1.078373000 -4.104235000 -0.683145000

C 0.266785000 -1.052683000 -2.861445000

C 0.166089000 -0.654640000 -4.260631000

C -0.266785000 1.052683000 -2.861445000

C -0.166089000 0.654640000 -4.260631000

C -0.716600000 2.792257000 -1.129038000

C -1.078373000 4.104235000 -0.683145000

C -0.716600000 2.792257000 1.129038000

C -1.078373000 4.104235000 0.683145000

C -0.597734000 2.356709000 2.453148000

C 0.597734000 -2.356709000 2.453148000

C 0.597734000 -2.356709000 -2.453148000

C -0.597734000 2.356709000 -2.453148000

C -0.887429000 3.373655000 3.517120000

C 0.887429000 -3.373655000 3.517120000

C 0.887429000 -3.373655000 -3.517120000

C -0.887429000 3.373655000 -3.517120000

H 1.304563000 -4.930524000 -1.334976000

H 1.304563000 -4.930524000 1.334976000

H 0.327047000 -1.294636000 5.112207000

H -0.327047000 1.294636000 5.112207000

H -1.304563000 4.930524000 1.334976000

H -1.304563000 4.930524000 -1.334976000

H -0.327047000 1.294636000 -5.112207000

H 0.327047000 -1.294636000 -5.112207000

C 0.088335000 4.220011000 4.056109000

C -2.192944000 3.500136000 4.010509000

C -0.217594000 5.152883000 5.044472000

C -2.513836000 4.426224000 4.996396000

H -3.531750000 4.498764000 5.357643000

H -2.959690000 2.851598000 3.605473000

C 2.192944000 -3.500136000 4.010509000

C -0.088335000 -4.220011000 4.056109000

C 2.513836000 -4.426224000 4.996396000

C 0.217594000 -5.152883000 5.044472000

H 2.959690000 -2.851598000 3.605473000

H 3.531750000 -4.498764000 5.357643000

C -0.088335000 -4.220011000 -4.056109000

C 2.192944000 -3.500136000 -4.010509000

C 0.217594000 -5.152883000 -5.044472000

C 2.513836000 -4.426224000 -4.996396000

H 3.531750000 -4.498764000 -5.357643000

H 2.959690000 -2.851598000 -3.605473000

C -2.192944000 3.500136000 -4.010509000

C 0.088335000 4.220011000 -4.056109000

C -2.513836000 4.426224000 -4.996396000

C -0.217594000 5.152883000 -5.044472000

H -2.959690000 2.851598000 -3.605473000

H -3.531750000 4.498764000 -5.357643000

C -1.522466000 5.254900000 -5.514361000

C -1.522466000 5.254900000 5.514361000

C 1.522466000 -5.254900000 5.514361000

C 1.522466000 -5.254900000 -5.514361000

H 0.236492000 -1.065234000 0.000000000

H -0.236492000 1.065234000 0.000000000

H 1.758404000 -5.980237000 -6.282927000

H 1.758404000 -5.980237000 6.282927000

H -1.758404000 5.980237000 6.282927000

H -1.758404000 5.980237000 -6.282927000

H 0.561033000 5.790314000 -5.439948000

H -0.561033000 -5.790314000 -5.439948000

H -0.561033000 -5.790314000 5.439948000

H 0.561033000 5.790314000 5.439948000

Br 1.903640000 4.124916000 3.453389000

Br 1.903640000 4.124916000 -3.453389000

Br -1.903640000 -4.124916000 -3.453389000

Br -1.903640000 -4.124916000 3.453389000

78

o-IV o-4C6H4Br-H2P

N 0.503760000 1.974715000 0.000000000

N 0.000000000 0.000000000 2.101878000

N -0.503760000 -1.974715000 0.000000000

N 0.000000000 0.000000000 -2.101878000

C 0.706028000 2.772785000 1.085974000

C 1.052246000 4.128438000 0.675381000

C 0.706028000 2.772785000 -1.085974000

C 1.052246000 4.128438000 -0.675381000

C 0.277385000 1.094423000 -2.882935000

C 0.168664000 0.661982000 -4.243902000

C -0.277385000 -1.094423000 -2.882935000

C -0.168664000 -0.661982000 -4.243902000

C -0.706028000 -2.772785000 -1.085974000

C -1.052246000 -4.128438000 -0.675381000

C -0.706028000 -2.772785000 1.085974000

C -1.052246000 -4.128438000 0.675381000

C -0.277385000 -1.094423000 2.882935000

C -0.168664000 -0.661982000 4.243902000

C 0.277385000 1.094423000 2.882935000

C 0.168664000 0.661982000 4.243902000

C 0.599186000 2.378757000 2.431386000

C 0.599186000 2.378757000 -2.431386000

C -0.599186000 -2.378757000 -2.431386000

C -0.599186000 -2.378757000 2.431386000

C 0.882606000 3.404269000 3.488850000

C 0.882606000 3.404269000 -3.488850000

C -0.882606000 -3.404269000 -3.488850000

C -0.882606000 -3.404269000 3.488850000

H -0.328355000 -1.293888000 -5.100627000

H 0.328355000 1.293888000 -5.100627000

H 1.258381000 4.954663000 -1.335356000

H 1.258381000 4.954663000 1.335356000

H 0.328355000 1.293888000 5.100627000

H -0.328355000 -1.293888000 5.100627000

H -1.258381000 -4.954663000 1.335356000

H -1.258381000 -4.954663000 -1.335356000

C -0.104949000 4.222539000 4.049342000

C 2.194271000 3.567536000 3.954294000

C 0.196179000 5.165857000 5.029231000

C 2.510422000 4.504208000 4.931683000

H 3.533746000 4.606931000 5.269565000

H 2.970508000 2.942300000 3.531104000

C 2.194271000 3.567536000 -3.954294000

C -0.104949000 4.222539000 -4.049342000

C 2.510422000 4.504208000 -4.931683000

C 0.196179000 5.165857000 -5.029231000

H 2.970508000 2.942300000 -3.531104000

H 3.533746000 4.606931000 -5.269565000

C 0.104949000 -4.222539000 -4.049342000

C -2.194271000 -3.567536000 -3.954294000

C -0.196179000 -5.165857000 -5.029231000

C -2.510422000 -4.504208000 -4.931683000

H -3.533746000 -4.606931000 -5.269565000

H -2.970508000 -2.942300000 -3.531104000

C -2.194271000 -3.567536000 3.954294000

C 0.104949000 -4.222539000 4.049342000

C -2.510422000 -4.504208000 4.931683000

C -0.196179000 -5.165857000 5.029231000

H -2.970508000 -2.942300000 3.531104000

H -3.533746000 -4.606931000 5.269565000

C -1.507654000 -5.305652000 5.470128000

C 1.507654000 5.305652000 5.470128000

C 1.507654000 5.305652000 -5.470128000

C -1.507654000 -5.305652000 -5.470128000

H 0.000000000 0.000000000 -1.090452000

H 0.000000000 0.000000000 1.090452000

H -1.739976000 -6.039639000 -6.231549000

H 1.739976000 6.039639000 -6.231549000

H 1.739976000 6.039639000 6.231549000

H -1.739976000 -6.039639000 6.231549000

H 0.591011000 -5.782981000 5.439680000

H 0.591011000 -5.782981000 -5.439680000

H -0.591011000 5.782981000 -5.439680000

H -0.591011000 5.782981000 5.439680000

Br -1.928670000 4.079258000 3.482582000

Br 1.928670000 -4.079258000 3.482582000

Br 1.928670000 -4.079258000 -3.482582000

Br -1.928670000 4.079258000 -3.482582000

78

o-V o-4C6H4Br-H2P

N -2.038068000 0.000000000 -0.819807000

N 0.000000000 2.101894000 -0.818122000

N 2.038068000 0.000000000 -0.819807000

N 0.000000000 -2.101894000 -0.818122000

C -2.861336000 1.086001000 -0.814198000

C -4.260457000 0.675396000 -0.803868000

C -2.861336000 -1.086001000 -0.814198000

C -4.260457000 -0.675396000 -0.803868000

C -1.129060000 -2.882846000 -0.830390000

C -0.683146000 -4.243564000 -0.855223000

C 1.129060000 -2.882846000 -0.830390000

C 0.683146000 -4.243564000 -0.855223000

C 2.861336000 -1.086001000 -0.814198000

C 4.260457000 -0.675396000 -0.803868000

C 2.861336000 1.086001000 -0.814198000

C 4.260457000 0.675396000 -0.803868000

C 1.129060000 2.882846000 -0.830390000

C 0.683146000 4.243564000 -0.855223000

C -1.129060000 2.882846000 -0.830390000

C -0.683146000 4.243564000 -0.855223000

C -2.453160000 2.431450000 -0.818251000

C -2.453160000 -2.431450000 -0.818251000

C 2.453160000 -2.431450000 -0.818251000

C 2.453160000 2.431450000 -0.818251000

C -3.517215000 3.488547000 -0.844762000

C -3.517215000 -3.488547000 -0.844762000

C 3.517215000 -3.488547000 -0.844762000

C 3.517215000 3.488547000 -0.844762000

H 1.334995000 -5.100148000 -0.867384000

H -1.334995000 -5.100148000 -0.867384000

H -5.111880000 -1.335421000 -0.792213000

H -5.111880000 1.335421000 -0.792213000

H -1.334995000 5.100148000 -0.867384000

H 1.334995000 5.100148000 -0.867384000

H 5.111880000 1.335421000 -0.792213000

H 5.111880000 -1.335421000 -0.792213000

C -4.052630000 4.067813000 0.311557000

C -4.013910000 3.933572000 -2.077214000

C -5.041352000 5.047272000 0.247706000

C -5.000002000 4.910232000 -2.156967000

H -5.363753000 5.232157000 -3.124441000

H -3.611011000 3.494807000 -2.981520000

C -4.013910000 -3.933572000 -2.077214000

C -4.052630000 -4.067813000 0.311557000

C -5.000002000 -4.910232000 -2.156967000

C -5.041352000 -5.047272000 0.247706000

H -3.611011000 -3.494807000 -2.981520000

H -5.363753000 -5.232157000 -3.124441000

C 4.052630000 -4.067813000 0.311557000

C 4.013910000 -3.933572000 -2.077214000

C 5.041352000 -5.047272000 0.247706000

C 5.000002000 -4.910232000 -2.156967000

H 5.363753000 -5.232157000 -3.124441000

H 3.611011000 -3.494807000 -2.981520000

C 4.013910000 3.933572000 -2.077214000

C 4.052630000 4.067813000 0.311557000

C 5.000002000 4.910232000 -2.156967000

C 5.041352000 5.047272000 0.247706000

H 3.611011000 3.494807000 -2.981520000

H 5.363753000 5.232157000 -3.124441000

C 5.514811000 5.468298000 -0.990184000

C -5.514811000 5.468298000 -0.990184000

C -5.514811000 -5.468298000 -0.990184000

C 5.514811000 -5.468298000 -0.990184000

H 0.000000000 -1.090686000 -0.796922000

H 0.000000000 1.090686000 -0.796922000

H 6.283559000 -6.229396000 -1.037518000

H -6.283559000 -6.229396000 -1.037518000

H -6.283559000 6.229396000 -1.037518000

H 6.283559000 6.229396000 -1.037518000

H 5.434314000 5.472678000 1.160715000

H 5.434314000 -5.472678000 1.160715000

H -5.434314000 -5.472678000 1.160715000

H -5.434314000 5.472678000 1.160715000

Br -3.444862000 3.527549000 2.044695000

Br 3.444862000 3.527549000 2.044695000

Br 3.444862000 -3.527549000 2.044695000

Br -3.444862000 -3.527549000 2.044695000