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Complex B1, ground state, CH<sub>2</sub>Cl<sub>2</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ir | 0.06065700  | 0.12516400  | -0.00432700 |
| N  | -2.03653600 | 0.40859200  | -0.01781800 |
| N  | 2.16844100  | -0.02708200 | 0.18177100  |
| O  | -7.09816400 | -0.07303900 | -0.71331500 |
| O  | 6.88407500  | 1.52670300  | 0.13285800  |
| O  | -6.72510500 | -0.15956100 | 1.50707900  |
| C  | -2.63645800 | -0.08094700 | 1.08849300  |
| C  | 0.53022200  | 2.04084500  | 0.35873500  |
| C  | -0.36260800 | -0.28282500 | 1.91503000  |
| C  | 2.78637600  | 1.17308600  | 0.18120000  |
| C  | -4.98745500 | 1.45026900  | -2.06174800 |
| H  | -6.06489400 | 1.36188600  | -2.05253400 |
| C  | -1.74588100 | -0.44952000 | 2.18512500  |
| C  | -4.24832600 | 0.86489100  | -1.00016200 |
| O  | 7.19332600  | -0.52149600 | -0.75328800 |
| C  | -4.35105300 | 2.12776800  | -3.07961700 |
| H  | -4.93470400 | 2.57741500  | -3.87744000 |
| C  | 2.30645500  | -2.42880800 | 0.42951300  |
| H  | 1.24015400  | -2.44267100 | 0.58566900  |
| C  | 4.19525300  | 1.26646300  | 0.06301200  |
| H  | 4.65324600  | 2.24417900  | 0.01694200  |
| C  | 4.36395600  | -1.14229500 | 0.07724300  |
| C  | 1.91848300  | 2.33571700  | 0.31571100  |
| C  | -0.34831900 | 3.11631200  | 0.58879900  |
| H  | -1.41723000 | 2.93609200  | 0.65153700  |
| C  | -2.81462800 | 0.95910500  | -1.02233800 |
| C  | -4.04625000 | -0.19101200 | 1.16354700  |
| H  | -4.49244100 | -0.63538700 | 2.04184300  |
| C  | 4.98312600  | 0.14609100  | -0.03308000 |
| C  | 2.39235400  | 3.65550700  | 0.44710400  |
| H  | 3.45541000  | 3.87343300  | 0.40437700  |
| C  | 1.49663400  | 4.69811800  | 0.65009100  |
| H  | 1.85982700  | 5.71616800  | 0.75695400  |
| C  | 2.93470700  | -1.17970200 | 0.21406700  |
| C  | 0.12429100  | 4.42140700  | 0.72942900  |
| H  | -0.57913700 | 5.23252600  | 0.90365000  |
| C  | -2.19451300 | 1.67657500  | -2.07417500 |
| H  | -1.11969000 | 1.77231600  | -2.06492600 |
| C  | 3.03920800  | -3.59579100 | 0.47343600  |
| H  | 2.53268400  | -4.53995500 | 0.65153900  |
| C  | 0.53946200  | -0.50861900 | 2.96888700  |
| H  | 1.60461400  | -0.37280200 | 2.80676300  |
| C  | -4.85204900 | 0.22678400  | 0.13256000  |
| C  | -2.94632900 | 2.25250300  | -3.07617300 |
| H  | -2.44899400 | 2.80854600  | -3.86556800 |
| C  | 5.08510100  | -2.36478100 | 0.10888400  |
| H  | 6.15902000  | -2.33443900 | -0.01238900 |
| C  | -6.33201300 | -0.00652500 | 0.23083500  |
| C  | -2.19344400 | -0.87678700 | 3.45039100  |
| H  | -3.25198200 | -1.01331600 | 3.65103200  |
| C  | 4.43795400  | -3.56738700 | 0.29754400  |
| H  | 5.00884100  | -4.49070100 | 0.32564200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.09068700  | -0.91906100 | 4.22523200  |
| H | 0.80897100  | -1.09009600 | 5.02377300  |
| C | 6.45734200  | 0.31394200  | -0.25978800 |
| C | -1.27637700 | -1.11435400 | 4.46747300  |
| H | -1.62015900 | -1.43892400 | 5.44529200  |
| C | 8.27909700  | 1.80722400  | -0.09772600 |
| H | 8.50527700  | 1.75744100  | -1.16546000 |
| H | 8.90293700  | 1.09047200  | 0.44107600  |
| H | 8.43688800  | 2.81584800  | 0.28199200  |
| C | -8.12412700 | -0.44617200 | 1.70434800  |
| H | -8.39584600 | -1.37709800 | 1.20127400  |
| H | -8.73586000 | 0.37095600  | 1.31528900  |
| H | -8.24979900 | -0.54042900 | 2.78217500  |
| S | 0.55553600  | -0.21014500 | -2.58362600 |
| C | -0.16475100 | -1.75476100 | -2.19866400 |
| C | -0.44602600 | -2.80052800 | -3.09871300 |
| C | -1.07459000 | -3.94499200 | -2.62820300 |
| H | -0.17963200 | -2.69162800 | -4.14468100 |
| C | -1.10493000 | -2.98254100 | -0.43538200 |
| C | -1.42212200 | -4.04336500 | -1.27189200 |
| H | -1.30283800 | -4.75852400 | -3.31127600 |
| H | -1.34041900 | -2.99899800 | 0.62505200  |
| H | -1.92204100 | -4.92034600 | -0.87591600 |
| N | -0.47979400 | -1.87852200 | -0.88271700 |

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Complex B2, ground state, CH2Cl2

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ir | 0.05862200  | 0.12379700  | 0.00540900  |
| N  | -2.04001300 | 0.40499000  | -0.01583200 |
| N  | 2.16470200  | -0.02756300 | 0.19705500  |
| O  | -7.09372700 | -0.10366000 | -0.73942500 |
| O  | 6.87935600  | 1.52506500  | 0.11402700  |
| O  | -6.73464200 | -0.17732400 | 1.48387600  |
| C  | -2.64334400 | -0.08781600 | 1.08719100  |
| C  | 0.52526200  | 2.03854000  | 0.37212500  |
| C  | -0.37237500 | -0.28615100 | 1.92399500  |
| C  | 2.78217500  | 1.17270800  | 0.19392000  |
| C  | -4.98432200 | 1.43317500  | -2.07581900 |
| H  | -6.06122200 | 1.33797000  | -2.07337300 |
| C  | -1.75652600 | -0.45548400 | 2.18745600  |
| C  | -4.24809100 | 0.85195600  | -1.00987100 |
| O  | 7.18079400  | -0.52436300 | -0.77212300 |
| C  | -4.34583300 | 2.11517600  | -3.08922300 |
| H  | -4.92711000 | 2.56125700  | -3.89071100 |
| C  | 2.30343400  | -2.42808600 | 0.45485700  |
| H  | 1.23972600  | -2.43944700 | 0.62920000  |
| C  | 4.19030900  | 1.26585100  | 0.06779900  |
| H  | 4.64827100  | 2.24345700  | 0.01863900  |
| C  | 4.35830500  | -1.14341400 | 0.07980700  |
| C  | 1.91339600  | 2.33413200  | 0.33194000  |
| C  | -0.35496500 | 3.11154200  | 0.60463700  |
| H  | -1.42372800 | 2.93005500  | 0.66502600  |
| C  | -2.81489800 | 0.95414500  | -1.02365500 |
| C  | -4.05308100 | -0.20301600 | 1.15514700  |
| H  | -4.50226800 | -0.64904600 | 2.03107000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 4.97675200  | 0.14495200  | -0.03527400 |
| C | 2.38590600  | 3.65361100  | 0.46955500  |
| H | 3.44896000  | 3.87210900  | 0.43028900  |
| C | 1.48881500  | 4.69456400  | 0.67526000  |
| H | 1.85092500  | 5.71243100  | 0.78705900  |
| C | 2.93036200  | -1.18029700 | 0.22811700  |
| C | 0.11666200  | 4.41649400  | 0.75100600  |
| H | -0.58776200 | 5.22629800  | 0.92700200  |
| C | -2.19292900 | 1.67805300  | -2.06992600 |
| H | -1.11937900 | 1.78584500  | -2.05147800 |
| C | 3.03577800  | -3.59546800 | 0.49465900  |
| H | 2.53119300  | -4.53868500 | 0.68273900  |
| C | 0.52531200  | -0.51006700 | 2.98156000  |
| H | 1.59091900  | -0.37218100 | 2.82428000  |
| C | -4.85479400 | 0.21112600  | 0.11948200  |
| C | -2.94203200 | 2.25010400  | -3.07605300 |
| H | -2.44343500 | 2.81131300  | -3.86090500 |
| C | 5.07879400  | -2.36642400 | 0.10643500  |
| H | 6.15155000  | -2.33705400 | -0.02480300 |
| C | -6.33449500 | -0.02880800 | 0.20955600  |
| C | -2.20907000 | -0.88366200 | 3.45057600  |
| H | -3.26821200 | -1.02202900 | 3.64652100  |
| C | 4.43253400  | -3.56821800 | 0.30320800  |
| H | 5.00297900  | -4.49186900 | 0.32728000  |
| C | 0.07153000  | -0.92115100 | 4.23606400  |
| H | 0.78645400  | -1.09044400 | 5.03793000  |
| C | 6.44939900  | 0.31216800  | -0.27382000 |
| C | -1.29610400 | -1.11917700 | 4.47189100  |
| H | -1.64376900 | -1.44422000 | 5.44815400  |
| C | 8.27270700  | 1.80514600  | -0.12790100 |
| H | 8.49032300  | 1.75370500  | -1.19731300 |
| H | 8.90054000  | 1.08903600  | 0.40706900  |
| H | 8.43343800  | 2.81429700  | 0.24910900  |
| C | -8.13375000 | -0.46916000 | 1.67406200  |
| H | -8.39795900 | -1.40417000 | 1.17461600  |
| H | -8.74650200 | 0.34299000  | 1.27635200  |
| H | -8.26568700 | -0.55774000 | 2.75160000  |
| S | 0.55978900  | -0.20040900 | -2.56573900 |
| C | -0.14050900 | -1.74732100 | -2.20001500 |
| C | -1.10499700 | -2.99121300 | -0.48693100 |
| C | -0.96045800 | -3.81608800 | -2.70329600 |
| C | -1.38332100 | -4.01453700 | -1.38570700 |
| H | -1.37491900 | -3.05016600 | 0.56401200  |
| H | -1.12288000 | -4.58427300 | -3.45742000 |
| H | -1.89046000 | -4.92008700 | -1.07571500 |
| N | -0.47187400 | -1.87965200 | -0.88066400 |
| N | -0.35195500 | -2.70209800 | -3.12036600 |

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Complex B3, ground state, CH2Cl2

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ir | -0.29360400 | -0.50129300 | 0.00088900  |
| N  | 1.75685000  | -1.02904600 | -0.04036200 |
| N  | -2.36921800 | -0.11926600 | 0.20114700  |
| O  | 6.84699300  | -1.10098500 | -0.68297400 |
| O  | -7.23096100 | -1.09595300 | -0.03597300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 6.45931900  | -1.18883300 | 1.53509500  |
| C | 2.39790300  | -0.71763700 | 1.10646900  |
| C | -0.98616000 | -2.37314400 | 0.19133500  |
| C | 0.15444700  | -0.32739500 | 1.94875900  |
| C | -3.12307200 | -1.23316800 | 0.08829200  |
| C | 4.58480700  | -2.22412400 | -2.17172500 |
| H | 5.66487900  | -2.26783700 | -2.15309600 |
| C | 1.54459400  | -0.34755500 | 2.23191300  |
| C | 3.90867100  | -1.65598100 | -1.05993500 |
| O | -7.28193000 | 1.04981900  | -0.72075200 |
| C | 3.88385300  | -2.71995300 | -3.25001400 |
| H | 4.41854600  | -3.15967700 | -4.08666700 |
| C | -2.22830500 | 2.24989600  | 0.66734700  |
| H | -1.17083500 | 2.12399400  | 0.83441200  |
| C | -4.53082000 | -1.14885400 | -0.04705800 |
| H | -5.09908900 | -2.05751800 | -0.18527800 |
| C | -4.41580900 | 1.25233300  | 0.18445900  |
| C | -2.39850300 | -2.49712100 | 0.11971400  |
| C | -0.24039600 | -3.55879000 | 0.32461700  |
| H | 0.84142500  | -3.51045200 | 0.40439000  |
| C | 2.47456400  | -1.57282600 | -1.09211500 |
| C | 3.80953400  | -0.78734900 | 1.19276800  |
| H | 4.29609000  | -0.48454900 | 2.10907800  |
| C | -5.17960300 | 0.06139500  | -0.04763100 |
| C | -3.02399800 | -3.75880900 | 0.13135500  |
| H | -4.10465300 | -3.84672700 | 0.06852900  |
| C | -2.25765300 | -4.91279500 | 0.24100100  |
| H | -2.73809900 | -5.88677700 | 0.25568300  |
| C | -2.99484100 | 1.10834500  | 0.33438400  |
| C | -0.86364500 | -4.80711100 | 0.34644200  |
| H | -0.26154200 | -5.70718600 | 0.44764800  |
| C | 1.78537400  | -2.10617300 | -2.20837800 |
| H | 0.70667300  | -2.07162100 | -2.21016300 |
| C | -2.82014300 | 3.48667800  | 0.81209900  |
| H | -2.21022400 | 4.34445500  | 1.08010600  |
| C | -0.72813100 | -0.10040300 | 3.01809400  |
| H | -1.79993000 | -0.09987900 | 2.84332600  |
| C | 4.57089900  | -1.20423900 | 0.12820300  |
| C | 2.47438000  | -2.67187200 | -3.26005500 |
| H | 1.92332800  | -3.08556200 | -4.09956100 |
| C | -4.98907200 | 2.54398600  | 0.32073900  |
| H | -6.05654800 | 2.65200100  | 0.18803800  |
| C | 6.06724500  | -1.16532600 | 0.25000400  |
| C | 2.02440700  | -0.09288900 | 3.53141700  |
| H | 3.08937100  | -0.09672900 | 3.74363900  |
| C | -4.20903800 | 3.63977800  | 0.62301300  |
| H | -4.66803800 | 4.61799600  | 0.73021700  |
| C | -0.24844900 | 0.13703900  | 4.30733600  |
| H | -0.95086000 | 0.31303600  | 5.11871900  |
| C | -6.65867200 | 0.09036500  | -0.30353800 |
| C | 1.12928200  | 0.15247400  | 4.56607900  |
| H | 1.49736200  | 0.34399300  | 5.56975700  |
| C | -8.64329200 | -1.18852400 | -0.31000100 |
| H | -8.83711300 | -1.00483400 | -1.36934700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -9.19377200 | -0.46276100 | 0.29286600  |
| H | -8.92346600 | -2.20542000 | -0.03831400 |
| C | 7.88038700  | -1.09773300 | 1.76106400  |
| H | 8.26973800  | -0.16012500 | 1.35751300  |
| H | 8.39246500  | -1.93911000 | 1.28877700  |
| H | 8.00281700  | -1.13129300 | 2.84281600  |
| S | -0.72528700 | 0.13128200  | -2.54189200 |
| C | 0.17000700  | 1.52604600  | -2.02453800 |
| C | 0.58443100  | 2.60774200  | -2.83223200 |
| C | 1.34680200  | 3.61485700  | -2.27218400 |
| H | 0.31151500  | 2.62756600  | -3.88138100 |
| C | 1.24604900  | 2.46626800  | -0.16353700 |
| C | 1.69754200  | 3.54608000  | -0.91008300 |
| H | 1.68124700  | 4.45073900  | -2.87955500 |
| H | 1.47930600  | 2.36572200  | 0.89112800  |
| N | 0.49231100  | 1.49708600  | -0.70212200 |
| C | 2.52725300  | 4.62874500  | -0.29487900 |
| F | 1.91049800  | 5.83424000  | -0.36409000 |
| F | 3.71411500  | 4.77619900  | -0.93280200 |
| F | 2.79844700  | 4.39292200  | 1.00697800  |

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Complex B4, ground state, CH2C12

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ir | 0.05586000  | -0.17212100 | 0.01709100  |
| S  | 0.57721900  | 0.60291500  | -2.53878500 |
| S  | -0.58979500 | 3.50093200  | -2.67485700 |
| O  | 7.17925700  | 0.63445500  | -0.60375600 |
| O  | 6.87657000  | -1.53679300 | -0.08442200 |
| O  | -7.09505100 | 0.22919100  | -0.61889100 |
| O  | -6.72172900 | -0.08907400 | 1.58032500  |
| N  | -0.44592600 | 1.95851300  | -0.55745000 |
| N  | 2.15536400  | -0.03890100 | 0.21225600  |
| N  | -2.04229900 | -0.43770800 | -0.03452900 |
| C  | -0.14891300 | 1.99362600  | -1.82226600 |
| C  | 2.91128400  | 1.09875900  | 0.43615600  |
| C  | 2.27239500  | 2.29280400  | 0.84951300  |
| H  | 1.20253600  | 2.27778300  | 0.98824400  |
| C  | 2.99996800  | 3.43816100  | 1.09401900  |
| H  | 2.48841000  | 4.33789600  | 1.42356100  |
| C  | 4.40016500  | 3.44533500  | 0.92687500  |
| H  | 4.96559700  | 4.35331400  | 1.11418700  |
| C  | 5.05556000  | 2.29506500  | 0.54260700  |
| H  | 6.13016700  | 2.29079300  | 0.42426500  |
| C  | 4.34151900  | 1.09167700  | 0.30238200  |
| C  | 4.96910300  | -0.15654100 | -0.02005500 |
| C  | 6.44540200  | -0.27638400 | -0.26478400 |
| C  | 8.27363800  | -1.76796400 | -0.35417300 |
| H  | 8.43358500  | -2.82738400 | -0.15805700 |
| H  | 8.50407100  | -1.52932000 | -1.39512100 |
| H  | 8.89235500  | -1.15598100 | 0.30608900  |
| C  | 4.18885200  | -1.28261900 | -0.11675600 |
| H  | 4.65412400  | -2.23589800 | -0.32321300 |
| C  | 2.78005000  | -1.21898400 | 0.01268400  |
| C  | 1.91755900  | -2.39320300 | -0.04513900 |
| C  | 2.39696700  | -3.71318500 | -0.14734900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.45988600  | -3.91549600 | -0.24075800 |
| C | 1.50643600  | -4.77977700 | -0.11566000 |
| H | 1.87420600  | -5.79909500 | -0.18968600 |
| C | 0.13434700  | -4.52884400 | 0.02516200  |
| H | -0.56405500 | -5.36173900 | 0.06426000  |
| C | -0.34482300 | -3.22115400 | 0.11459800  |
| H | -1.41405300 | -3.05945900 | 0.21560900  |
| C | 0.52818000  | -2.11899100 | 0.06169400  |
| C | -2.82737300 | -0.79175000 | -1.11815200 |
| C | -2.21579700 | -1.31618300 | -2.28268000 |
| H | -1.14214000 | -1.42799800 | -2.29370500 |
| C | -2.97457700 | -1.69198300 | -3.37077900 |
| H | -2.48441600 | -2.10294300 | -4.24850700 |
| C | -4.37764000 | -1.55017300 | -3.34896800 |
| H | -4.96651200 | -1.84016400 | -4.21408300 |
| C | -5.00588800 | -1.05932500 | -2.22444300 |
| H | -6.08208000 | -0.95961200 | -2.19760900 |
| C | -4.25967200 | -0.68466900 | -1.07610600 |
| C | -4.85438300 | -0.25166800 | 0.15426400  |
| C | -6.33071700 | -0.01740800 | 0.29637400  |
| C | -8.11580000 | 0.18166400  | 1.82917400  |
| H | -8.24184900 | 0.07742500  | 2.90601900  |
| H | -8.36912400 | 1.19452300  | 1.50738400  |
| H | -8.74153700 | -0.53787600 | 1.29631700  |
| C | -4.04278500 | -0.03513500 | 1.24136800  |
| H | -4.48271400 | 0.25223300  | 2.18576100  |
| C | -2.63453300 | -0.14541700 | 1.14287900  |
| C | -1.73624800 | 0.02280000  | 2.27979900  |
| C | -2.17260800 | 0.21649800  | 3.60451100  |
| H | -3.23002100 | 0.30686300  | 3.83510500  |
| C | -1.24645500 | 0.27778800  | 4.63913700  |
| H | -1.58175500 | 0.42124900  | 5.66214500  |
| C | 0.11904100  | 0.13938600  | 4.35344800  |
| H | 0.84486000  | 0.17301500  | 5.16265300  |
| C | 0.55798200  | -0.04090400 | 3.04066400  |
| H | 1.62206000  | -0.13821900 | 2.84745900  |
| C | -0.35529500 | -0.08516100 | 1.97362600  |
| C | -0.97559400 | 4.28376400  | -1.04501000 |
| H | -0.11564500 | 4.88328200  | -0.73630200 |
| H | -1.84901200 | 4.92997700  | -1.14575500 |
| C | -1.22384000 | 3.10253100  | -0.08400000 |
| H | -2.28777600 | 2.82844800  | -0.06799500 |
| H | -0.93455000 | 3.36600800  | 0.93834400  |

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Complex B5, ground state, CH2Cl2

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ir | 0.17857800  | -0.42923300 | 0.00140300  |
| S  | 0.69974300  | 0.25970300  | -2.56846900 |
| S  | -0.47910800 | 3.13918500  | -2.84009300 |
| O  | 7.24610500  | 0.76331200  | -0.59825400 |
| O  | 7.06894900  | -1.39976900 | 0.00672600  |
| O  | -6.98524400 | -0.49470700 | -0.66402900 |
| O  | -6.60086800 | -0.77681300 | 1.53839200  |
| N  | -0.44733400 | 1.68324300  | -0.68055800 |
| N  | 2.26569500  | -0.17065200 | 0.21319700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -1.90194900 | -0.82134800 | -0.05705300 |
| C | -0.07868200 | 1.65888500  | -1.94957500 |
| C | -1.08489900 | 2.86328300  | -0.31913600 |
| C | -1.19654600 | 3.80252900  | -1.37261400 |
| C | -1.80168200 | 5.04428700  | -1.17981200 |
| H | -1.88382700 | 5.75771700  | -1.99398100 |
| C | -2.29922600 | 5.34745600  | 0.08877000  |
| H | -2.77435000 | 6.30882600  | 0.25998400  |
| C | -2.19165300 | 4.42421400  | 1.14054100  |
| H | -2.58569100 | 4.67976200  | 2.11995000  |
| C | -1.58773900 | 3.18277200  | 0.95050600  |
| H | -1.50810600 | 2.46581000  | 1.76092300  |
| C | 2.95342700  | 1.01443900  | 0.40783500  |
| C | 2.24446700  | 2.18066400  | 0.78224400  |
| H | 1.17793900  | 2.11005800  | 0.92629500  |
| C | 2.90179500  | 3.37481400  | 0.98853200  |
| H | 2.33565400  | 4.25251600  | 1.28627400  |
| C | 4.29975000  | 3.45884800  | 0.82306900  |
| H | 4.80996000  | 4.40459100  | 0.97928900  |
| C | 5.02331800  | 2.33650000  | 0.48088500  |
| H | 6.09684300  | 2.39140500  | 0.36570400  |
| C | 4.38217500  | 1.08574800  | 0.27986300  |
| C | 5.08245400  | -0.13429800 | 0.00377900  |
| C | 6.56553600  | -0.17576800 | -0.22700100 |
| C | 8.47978100  | -1.55750200 | -0.24439000 |
| H | 8.70050600  | -2.59698300 | -0.00547200 |
| H | 8.70471800  | -1.34623400 | -1.29237100 |
| H | 9.05499100  | -0.88436700 | 0.39531200  |
| C | 4.36908800  | -1.30631900 | -0.06076200 |
| H | 4.88994300  | -2.23767400 | -0.23144700 |
| C | 2.95754300  | -1.31821000 | 0.05407700  |
| C | 2.16109000  | -2.53919200 | 0.02216900  |
| C | 2.71208400  | -3.83335600 | -0.03404300 |
| H | 3.78559900  | -3.97949500 | -0.10760900 |
| C | 1.88038400  | -4.94574500 | 0.01926700  |
| H | 2.30410400  | -5.94503500 | -0.01895200 |
| C | 0.49531100  | -4.76627800 | 0.13586600  |
| H | -0.15752200 | -5.63425600 | 0.19229500  |
| C | -0.05596700 | -3.48465600 | 0.18051800  |
| H | -1.13319400 | -3.37923000 | 0.26537400  |
| C | 0.75758900  | -2.34019000 | 0.10427700  |
| C | -2.65835500 | -1.24166900 | -1.13769200 |
| C | -2.01058000 | -1.74786900 | -2.29043800 |
| H | -0.93233800 | -1.79530600 | -2.29539200 |
| C | -2.73921700 | -2.18978900 | -3.37426800 |
| H | -2.22009700 | -2.58569400 | -4.24220300 |
| C | -4.14840100 | -2.13611500 | -3.35975800 |
| H | -4.71411200 | -2.47809000 | -4.22129000 |
| C | -4.81090300 | -1.66732400 | -2.24561400 |
| H | -5.89135500 | -1.63655000 | -2.22323700 |
| C | -4.09462500 | -1.22695800 | -1.10151900 |
| C | -4.72080800 | -0.81814400 | 0.12098100  |
| C | -6.21042700 | -0.68379100 | 0.25597100  |
| C | -8.01182600 | -0.60525100 | 1.78021100  |

|   |             |             |            |
|---|-------------|-------------|------------|
| H | -8.13498000 | -0.71406200 | 2.85690300 |
| H | -8.33546100 | 0.38557900  | 1.45300800 |
| H | -8.58181800 | -1.36991200 | 1.24766800 |
| C | -3.92940400 | -0.53545500 | 1.20754000 |
| H | -4.39100200 | -0.26726800 | 2.14723400 |
| C | -2.51673800 | -0.55488000 | 1.11434500 |
| C | -1.63649300 | -0.31909200 | 2.25428100 |
| C | -2.09092000 | -0.13596700 | 3.57438500 |
| H | -3.15288900 | -0.11125400 | 3.79980900 |
| C | -1.17523200 | 0.00025500  | 4.61176700 |
| H | -1.52442000 | 0.13614300  | 5.63110000 |
| C | 0.19738100  | -0.05313900 | 4.33381200 |
| H | 0.91555600  | 0.03891800  | 5.14519100 |
| C | 0.65328200  | -0.22236700 | 3.02504700 |
| H | 1.72213800  | -0.25354300 | 2.83703600 |
| C | -0.25010900 | -0.33913300 | 1.95604800 |

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Complex B1, excited state, CH2Cl2

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ir | 0.07346200  | 0.17496600  | -0.02916600 |
| N  | -1.99383700 | 0.52365900  | 0.04151100  |
| N  | 2.21609100  | -0.05751700 | 0.08384300  |
| O  | -7.16208700 | 0.40385500  | -0.36904700 |
| O  | 6.95522700  | 1.37009000  | 0.33664600  |
| O  | -6.57859500 | -0.58803000 | 1.57651100  |
| C  | -2.58442200 | -0.03075200 | 1.16497100  |
| C  | 0.61206600  | 2.04659700  | 0.32866800  |
| C  | -0.26089500 | -0.42479800 | 1.85453000  |
| C  | 2.86045300  | 1.12148500  | 0.16199500  |
| C  | -5.00112900 | 1.59451200  | -1.89237500 |
| H  | -6.07677700 | 1.49502100  | -1.84891100 |
| C  | -1.64382100 | -0.47368800 | 2.19311800  |
| C  | -4.24438900 | 0.99490000  | -0.86046600 |
| O  | 7.26556200  | -0.59792600 | -0.71631800 |
| C  | -4.40263500 | 2.29859500  | -2.93004800 |
| H  | -5.01941600 | 2.74720900  | -3.70425400 |
| C  | 2.28108800  | -2.47353700 | 0.04427300  |
| H  | 1.20644400  | -2.47849100 | 0.13139500  |
| C  | 4.27176000  | 1.19350400  | 0.09813200  |
| H  | 4.75436000  | 2.15906300  | 0.14396700  |
| C  | 4.38478800  | -1.21257100 | -0.07434400 |
| C  | 2.01279900  | 2.30043300  | 0.32336400  |
| C  | -0.26041500 | 3.13338700  | 0.54796100  |
| H  | -1.33049100 | 2.96504000  | 0.57153200  |
| C  | -2.80856600 | 1.10613100  | -0.92259200 |
| C  | -3.95769900 | -0.15163700 | 1.27413900  |
| H  | -4.37315000 | -0.62047600 | 2.15543600  |
| C  | 5.03664400  | 0.06126400  | -0.04466400 |
| C  | 2.50493600  | 3.60101000  | 0.49917600  |
| H  | 3.57073900  | 3.80379200  | 0.48974400  |
| C  | 1.61838900  | 4.65807800  | 0.70100300  |
| H  | 2.00315100  | 5.66396100  | 0.83951600  |
| C  | 2.94889300  | -1.22623000 | 0.00923900  |
| C  | 0.23755500  | 4.42139200  | 0.73258500  |
| H  | -0.44812600 | 5.24713300  | 0.90142800  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.23292600 | 1.85798500  | -1.97008600 |
| H | -1.15874100 | 1.97193000  | -1.99602900 |
| C | 2.98514500  | -3.65632500 | -0.01552700 |
| H | 2.44975400  | -4.60041100 | 0.02007700  |
| C | 0.70021400  | -0.79900100 | 2.80957000  |
| H | 1.75562900  | -0.76595700 | 2.56111500  |
| C | -4.83577900 | 0.29622700  | 0.27004200  |
| C | -3.01051800 | 2.44065400  | -2.96135800 |
| H | -2.53040500 | 3.00873300  | -3.75379500 |
| C | 5.07590700  | -2.45096900 | -0.14385500 |
| H | 6.15410500  | -2.43763300 | -0.21902900 |
| C | -6.26988500 | 0.07348600  | 0.41430800  |
| C | -2.01750400 | -0.88925800 | 3.48310800  |
| H | -3.06360300 | -0.90782700 | 3.77267100  |
| C | 4.39230200  | -3.64701700 | -0.11660600 |
| H | 4.93926700  | -4.58363900 | -0.16531600 |
| C | 0.31277600  | -1.21535500 | 4.08213800  |
| H | 1.06272800  | -1.50053400 | 4.81459500  |
| C | 6.52663500  | 0.20974400  | -0.18451000 |
| C | -1.04957300 | -1.26296900 | 4.41282100  |
| H | -1.35640300 | -1.58598000 | 5.40385700  |
| C | 8.36677400  | 1.63712100  | 0.20289800  |
| H | 8.64584500  | 1.67687900  | -0.85246500 |
| H | 8.94638600  | 0.85993500  | 0.70579100  |
| H | 8.52308900  | 2.60371900  | 0.67962200  |
| C | -7.96974200 | -0.84278300 | 1.78993600  |
| H | -8.38062400 | -1.47248400 | 0.99508800  |
| H | -8.53943700 | 0.09045800  | 1.83040100  |
| H | -8.02953100 | -1.36115300 | 2.74814700  |
| S | 0.45427800  | -0.21824500 | -2.54274700 |
| C | -0.44884400 | -1.68142300 | -2.20674800 |
| C | -0.91272300 | -2.62460300 | -3.13654000 |
| C | -1.64606100 | -3.70904700 | -2.66945500 |
| H | -0.70602600 | -2.49136600 | -4.19287700 |
| C | -1.40752800 | -2.86979300 | -0.43556500 |
| C | -1.90533800 | -3.83860100 | -1.29763400 |
| H | -2.02067300 | -4.45114500 | -3.36855800 |
| H | -1.56968400 | -2.91561200 | 0.63655600  |
| H | -2.47650800 | -4.67291700 | -0.90624800 |
| N | -0.68657200 | -1.82735900 | -0.88245000 |

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Complex B2, excited state, CH2Cl2

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ir | 0.08516400  | 0.17348900  | 0.03518700  |
| N  | -2.04905900 | 0.44376900  | 0.02601500  |
| N  | 2.15741600  | -0.05601600 | 0.24502800  |
| O  | -7.09007400 | -0.10201800 | -0.73094400 |
| O  | 6.83857400  | 1.57046000  | -0.14250200 |
| O  | -6.72323000 | -0.31356600 | 1.48308500  |
| C  | -2.63649300 | -0.17061500 | 1.07050500  |
| C  | 0.55512600  | 2.02040900  | 0.52789800  |
| C  | -0.34719700 | -0.51324900 | 1.86998900  |
| C  | 2.83077400  | 1.15865800  | 0.32831400  |
| C  | -5.01184400 | 1.56665500  | -1.95047100 |
| H  | -6.08668300 | 1.45170300  | -1.95497700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.73680000 | -0.66191000 | 2.11960200  |
| C | -4.26291800 | 0.92242200  | -0.93031600 |
| O | 7.28031300  | -0.63566000 | -0.35197000 |
| C | -4.38622700 | 2.32931800  | -2.91214800 |
| H | -4.97578100 | 2.82131200  | -3.67972800 |
| C | 2.26367800  | -2.47367800 | 0.29602700  |
| H | 1.20018700  | -2.48923500 | 0.47474700  |
| C | 4.20746700  | 1.23619300  | 0.20390900  |
| H | 4.68115500  | 2.20725700  | 0.24851100  |
| C | 4.34129500  | -1.19116400 | 0.03245900  |
| C | 1.96442200  | 2.30031400  | 0.55006900  |
| C | -0.35013800 | 3.07480700  | 0.80198500  |
| H | -1.41642400 | 2.87668600  | 0.81292800  |
| C | -2.83050600 | 1.05279000  | -0.93672600 |
| C | -4.04189500 | -0.31261500 | 1.13600600  |
| H | -4.48281800 | -0.84318600 | 1.96757400  |
| C | 5.00978200  | 0.10178300  | 0.00708300  |
| C | 2.40977900  | 3.60966400  | 0.80096200  |
| H | 3.47061200  | 3.83782600  | 0.82153400  |
| C | 1.49162900  | 4.62545400  | 1.04337100  |
| H | 1.84803000  | 5.63320400  | 1.23788600  |
| C | 2.90577500  | -1.22028300 | 0.18250400  |
| C | 0.10681200  | 4.36006000  | 1.05286700  |
| H | -0.59645800 | 5.16202900  | 1.25785900  |
| C | -2.22244800 | 1.86152500  | -1.92863800 |
| H | -1.15091300 | 1.98963800  | -1.91021700 |
| C | 2.96756400  | -3.66683900 | 0.20924800  |
| H | 2.43736200  | -4.61086900 | 0.30099000  |
| C | 0.56200500  | -0.89157000 | 2.87032500  |
| H | 1.62732000  | -0.78674300 | 2.69803100  |
| C | -4.85339500 | 0.18382500  | 0.14330300  |
| C | -2.98400500 | 2.48719000  | -2.89153600 |
| H | -2.49771600 | 3.11012900  | -3.63617800 |
| C | 5.01999700  | -2.42367800 | -0.06256700 |
| H | 6.09286200  | -2.39750600 | -0.19280700 |
| C | -6.33214600 | -0.07966800 | 0.22082500  |
| C | -2.18494800 | -1.18870100 | 3.34144000  |
| H | -3.24442700 | -1.29870900 | 3.54850300  |
| C | 4.35225800  | -3.64264500 | 0.01437300  |
| H | 4.91376600  | -4.56975800 | -0.06229900 |
| C | 0.10722300  | -1.40536300 | 4.08603600  |
| H | 0.82214800  | -1.68807500 | 4.85396600  |
| C | 6.44920600  | 0.25663700  | -0.17732600 |
| C | -1.26416500 | -1.56034800 | 4.31944400  |
| H | -1.61573900 | -1.96478100 | 5.26385700  |
| C | 8.23988800  | 1.80287600  | -0.31416300 |
| H | 8.58356800  | 1.43129600  | -1.28402200 |
| H | 8.81849800  | 1.31531900  | 0.47606600  |
| H | 8.36642000  | 2.88510300  | -0.25983600 |
| C | -8.11922200 | -0.63179200 | 1.66182000  |
| H | -8.37413100 | -1.53913800 | 1.10956400  |
| H | -8.74162700 | 0.19564700  | 1.31417700  |
| H | -8.24454900 | -0.78428600 | 2.73281400  |
| S | 0.60204000  | 0.04949900  | -2.52032000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.16880100 | -1.49802200 | -2.32916200 |
| C | -1.16003400 | -2.88860600 | -0.75559900 |
| C | -1.05129000 | -3.46799700 | -3.05211900 |
| C | -1.46613600 | -3.80010900 | -1.75903900 |
| H | -1.42594100 | -3.05682900 | 0.28406800  |
| H | -1.24271300 | -4.14189800 | -3.88489200 |
| H | -1.99080000 | -4.72309700 | -1.54476800 |
| N | -0.50216700 | -1.75631600 | -1.03385200 |
| N | -0.41398000 | -2.33111300 | -3.34895500 |

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Complex B3, excited state, CH2Cl2

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ir | -0.33688000 | -0.52810600 | 0.02480600  |
| N  | 1.66388300  | -1.14766500 | 0.01811200  |
| N  | -2.43403100 | -0.03114200 | 0.16020300  |
| O  | 6.79066400  | -1.68445200 | -0.52443000 |
| O  | -7.31645200 | -0.87711700 | 0.08624300  |
| O  | 6.38509000  | -0.74392600 | 1.48975100  |
| C  | 2.34396600  | -0.75916600 | 1.16405300  |
| C  | -1.10698900 | -2.33650500 | 0.25227900  |
| C  | 0.10084500  | -0.13317100 | 1.92967300  |
| C  | -3.21971700 | -1.12298800 | 0.12090700  |
| C  | 4.46114300  | -2.48033900 | -2.05566100 |
| H  | 5.54111100  | -2.52610700 | -2.03786900 |
| C  | 1.48675600  | -0.27975800 | 2.24097400  |
| C  | 3.81261900  | -1.85510300 | -0.96878900 |
| O  | -7.33195500 | 1.20057500  | -0.78633700 |
| C  | 3.75267700  | -3.03149400 | -3.11794600 |
| H  | 4.28940400  | -3.50619900 | -3.93493400 |
| C  | -2.20619000 | 2.36737100  | 0.35687600  |
| H  | -1.14693100 | 2.23112100  | 0.50445800  |
| C  | -4.62413300 | -1.01373200 | -0.00232400 |
| H  | -5.22121900 | -1.91224700 | -0.05947700 |
| C  | -4.43628100 | 1.39394700  | 0.02476700  |
| C  | -2.52868600 | -2.40831000 | 0.21216100  |
| C  | -0.38255500 | -3.53768100 | 0.40631600  |
| H  | 0.69982200  | -3.50928400 | 0.44872700  |
| C  | 2.37337700  | -1.77184700 | -0.99836700 |
| C  | 3.72429200  | -0.82618000 | 1.24164400  |
| H  | 4.21500600  | -0.47779600 | 2.14015500  |
| C  | -5.23767300 | 0.21331900  | -0.08390000 |
| C  | -3.18387800 | -3.64383700 | 0.29703400  |
| H  | -4.26649400 | -3.70889000 | 0.26588300  |
| C  | -2.44141800 | -4.81624600 | 0.43888800  |
| H  | -2.95315000 | -5.77143800 | 0.50771800  |
| C  | -3.01553500 | 1.22148800  | 0.16934400  |
| C  | -1.04266300 | -4.76091200 | 0.49989600  |
| H  | -0.47047900 | -5.67663400 | 0.61987700  |
| C  | 1.68085000  | -2.37485800 | -2.07203300 |
| H  | 0.60083900  | -2.34869100 | -2.07030200 |
| C  | -2.75825400 | 3.62951000  | 0.37540400  |
| H  | -2.11710200 | 4.49224400  | 0.52925500  |
| C  | -0.79464500 | 0.28958700  | 2.93064900  |
| H  | -1.84900400 | 0.40218200  | 2.70154700  |
| C  | 4.51331700  | -1.31374200 | 0.18674700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.35411000  | -2.98859600 | -3.11920900 |
| H | 1.78759500  | -3.43758800 | -3.93058000 |
| C | -4.96790000 | 2.71070300  | 0.03571900  |
| H | -6.03392200 | 2.83851700  | -0.08915100 |
| C | 5.96818000  | -1.28835400 | 0.30250500  |
| C | 1.92697000  | -0.00266500 | 3.54807300  |
| H | 2.97178000  | -0.12747700 | 3.81457200  |
| C | -4.14773800 | 3.80497400  | 0.20383500  |
| H | -4.57398000 | 4.80339300  | 0.21555300  |
| C | -0.34149200 | 0.56060300  | 4.21802100  |
| H | -1.03879400 | 0.88054100  | 4.98698900  |
| C | -6.72508000 | 0.26329200  | -0.30231700 |
| C | 1.02386700  | 0.41771300  | 4.52008800  |
| H | 1.38042000  | 0.63064200  | 5.52409100  |
| C | -8.74010200 | -0.95568800 | -0.13419400 |
| H | -8.96345400 | -0.86477600 | -1.19961900 |
| H | -9.25085400 | -0.16243600 | 0.41603500  |
| H | -9.03518100 | -1.93521200 | 0.23927200  |
| C | 7.80225600  | -0.68427700 | 1.67701600  |
| H | 8.27546900  | -0.07394400 | 0.90212200  |
| H | 8.24372600  | -1.68509300 | 1.65675100  |
| H | 7.94961800  | -0.22822300 | 2.65708400  |
| S | -0.65526800 | 0.09378500  | -2.48473800 |
| C | 0.36073900  | 1.42818900  | -2.02220800 |
| C | 0.89253600  | 2.42106300  | -2.86854000 |
| C | 1.72268000  | 3.38379700  | -2.32404700 |
| H | 0.65796600  | 2.41258500  | -3.92693500 |
| C | 1.45215500  | 2.35327000  | -0.16827100 |
| C | 2.01818900  | 3.35235800  | -0.94854200 |
| H | 2.15099000  | 4.15646600  | -2.95540500 |
| H | 1.64073400  | 2.28313300  | 0.89685100  |
| N | 0.63507500  | 1.43014800  | -0.69449400 |
| C | 2.91755300  | 4.39167700  | -0.35227200 |
| F | 2.40619700  | 5.63803600  | -0.49991400 |
| F | 4.13084000  | 4.40578900  | -0.95313800 |
| F | 3.12273300  | 4.19621000  | 0.96738700  |

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Complex B4, excited state, CH2Cl2

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ir | -0.07233300 | 0.21024500  | 0.09173700  |
| S  | -0.63714500 | -0.14558100 | -2.52644000 |
| S  | 0.48684700  | -2.99366300 | -3.16318800 |
| O  | -7.25415200 | -0.62036200 | -0.28806300 |
| O  | -6.80511300 | 1.59373300  | -0.32759600 |
| O  | 7.08803200  | -0.16453700 | -0.76379100 |
| O  | 6.75397100  | -0.19601200 | 1.46508200  |
| N  | 0.41521500  | -1.80818600 | -0.82657100 |
| N  | -2.14062400 | 0.00859300  | 0.31420100  |
| N  | 2.05909300  | 0.45654000  | 0.02105400  |
| C  | 0.09084800  | -1.64228800 | -2.07315900 |
| C  | -2.89144600 | -1.15386200 | 0.37452300  |
| C  | -2.25428300 | -2.38798600 | 0.63751600  |
| H  | -1.19063000 | -2.38550600 | 0.81980600  |
| C  | -2.96290500 | -3.58053100 | 0.68036300  |
| H  | -2.43868000 | -4.50990100 | 0.88597700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.34587900 | -3.57408600 | 0.47034300  |
| H | -4.91064700 | -4.50206500 | 0.49567700  |
| C | -5.00813800 | -2.37015500 | 0.24699900  |
| H | -6.07966100 | -2.35640600 | 0.10431200  |
| C | -4.32499800 | -1.13715700 | 0.20721300  |
| C | -4.98715500 | 0.14724500  | 0.02756800  |
| C | -6.42234400 | 0.28384200  | -0.20144000 |
| C | -8.20145300 | 1.80930300  | -0.55427900 |
| H | -8.32173200 | 2.89053500  | -0.63567200 |
| H | -8.52869100 | 1.32257600  | -1.47768900 |
| H | -8.79845900 | 1.42525700  | 0.27825300  |
| C | -4.18478400 | 1.29481500  | 0.11522500  |
| H | -4.65636100 | 2.26577400  | 0.04839500  |
| C | -2.80997500 | 1.22835900  | 0.26724900  |
| C | -1.94100900 | 2.38330500  | 0.38320500  |
| C | -2.38521900 | 3.71188900  | 0.50611700  |
| H | -3.44557300 | 3.94315100  | 0.49696400  |
| C | -1.46654700 | 4.74361000  | 0.65950200  |
| H | -1.82176600 | 5.76595400  | 0.75485800  |
| C | -0.08149200 | 4.47827500  | 0.70591900  |
| H | 0.62124900  | 5.29550200  | 0.84041000  |
| C | 0.37415600  | 3.17494100  | 0.58060500  |
| H | 1.44019600  | 2.97681400  | 0.61738300  |
| C | -0.53090300 | 2.09976200  | 0.40208000  |
| C | 2.82601100  | 0.97059100  | -1.00590200 |
| C | 2.20149400  | 1.68404200  | -2.05833800 |
| H | 1.12962200  | 1.80890000  | -2.03462100 |
| C | 2.94709300  | 2.21926800  | -3.08600600 |
| H | 2.44872900  | 2.77025800  | -3.87789300 |
| C | 4.34920500  | 2.06129400  | -3.11214700 |
| H | 4.92667500  | 2.48217900  | -3.92960600 |
| C | 4.99060900  | 1.38857900  | -2.09506500 |
| H | 6.06541800  | 1.27380000  | -2.10620500 |
| C | 4.25834700  | 0.83901300  | -1.00954300 |
| C | 4.86523500  | 0.19842200  | 0.11707400  |
| C | 6.34419500  | -0.06284100 | 0.19398300  |
| C | 8.15152500  | -0.50488100 | 1.64746400  |
| H | 8.29246100  | -0.57419500 | 2.72512300  |
| H | 8.39570600  | -1.45332900 | 1.16366900  |
| H | 8.77095100  | 0.29059700  | 1.22741500  |
| C | 4.06880100  | -0.20303500 | 1.16360500  |
| H | 4.52119300  | -0.65779000 | 2.03317400  |
| C | 2.66298800  | -0.06082200 | 1.10776900  |
| C | 1.77771200  | -0.44431300 | 2.20988500  |
| C | 2.23586300  | -0.86983000 | 3.46601700  |
| H | 3.29660200  | -0.98064300 | 3.66619400  |
| C | 1.32396000  | -1.13939700 | 4.48522300  |
| H | 1.68332300  | -1.46599100 | 5.45642900  |
| C | -0.04887200 | -0.98137800 | 4.25904500  |
| H | -0.75574200 | -1.18359100 | 5.05911100  |
| C | -0.51490900 | -0.56827200 | 3.01032800  |
| H | -1.58052600 | -0.45898700 | 2.84370100  |
| C | 0.38609900  | -0.29850100 | 1.96682400  |
| C | 0.89034700  | -4.03127600 | -1.68558800 |

|   |            |             |             |
|---|------------|-------------|-------------|
| H | 0.02408200 | -4.65659200 | -1.45731800 |
| H | 1.74857000 | -4.66661200 | -1.90923600 |
| C | 1.18195100 | -3.02387100 | -0.55418100 |
| H | 2.25089800 | -2.77329000 | -0.51869200 |
| H | 0.90475800 | -3.44101700 | 0.41851900  |

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Complex B5, excited state, CH2Cl2

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ir | 0.20124800  | -0.47577800 | 0.05700400  |
| S  | 0.76048400  | 0.07921100  | -2.51641600 |
| S  | -0.42007900 | 2.93035300  | -2.98399400 |
| O  | 7.30838100  | 0.84824300  | -0.18216000 |
| O  | 7.01159900  | -1.37988500 | -0.40634900 |
| O  | -6.97844400 | -0.43371300 | -0.70088200 |
| O  | -6.62084500 | -0.64570600 | 1.51465100  |
| N  | -0.42325500 | 1.60713300  | -0.74272200 |
| N  | 2.24526800  | -0.16112500 | 0.30794300  |
| N  | -1.91439200 | -0.85401600 | -0.02487900 |
| C  | -0.03385800 | 1.51253200  | -2.00135200 |
| C  | -1.06864300 | 2.80529800  | -0.45985000 |
| C  | -1.16365500 | 3.67750700  | -1.57075600 |
| C  | -1.77116200 | 4.92858500  | -1.46518000 |
| H  | -1.83924200 | 5.59017500  | -2.32308200 |
| C  | -2.28839000 | 5.30922100  | -0.22616800 |
| H  | -2.76568400 | 6.27900400  | -0.12224700 |
| C  | -2.19670700 | 4.45342200  | 0.88249800  |
| H  | -2.60431800 | 4.76923500  | 1.83833800  |
| C  | -1.59032800 | 3.20324100  | 0.77930000  |
| H  | -1.52119600 | 2.54229700  | 1.63644700  |
| C  | 2.91802200  | 1.03485600  | 0.48290500  |
| C  | 2.19955600  | 2.19606000  | 0.84990700  |
| H  | 1.13828100  | 2.11182600  | 1.02610200  |
| C  | 2.82767900  | 3.42469700  | 1.00121500  |
| H  | 2.24175400  | 4.29562300  | 1.28120200  |
| C  | 4.20768500  | 3.52626600  | 0.80269700  |
| H  | 4.71071100  | 4.48298100  | 0.91302200  |
| C  | 4.94963000  | 2.39096700  | 0.48073800  |
| H  | 6.01992500  | 2.46110500  | 0.34574300  |
| C  | 4.35026900  | 1.12600800  | 0.32748200  |
| C  | 5.09676800  | -0.09291100 | 0.04168600  |
| C  | 6.54084500  | -0.11426400 | -0.17987900 |
| C  | 8.42093700  | -1.48286100 | -0.63430700 |
| H  | 8.61537200  | -2.54471500 | -0.79135000 |
| H  | 8.71760600  | -0.91011300 | -1.51785900 |
| H  | 8.98549700  | -1.11925200 | 0.22921900  |
| C  | 4.37319400  | -1.29212800 | 0.01757300  |
| H  | 4.90794300  | -2.22061000 | -0.12906700 |
| C  | 2.99525600  | -1.33019300 | 0.15976700  |
| C  | 2.20313000  | -2.53930900 | 0.16434700  |
| C  | 2.72954400  | -3.84555400 | 0.16085800  |
| H  | 3.80213900  | -4.00766100 | 0.13151700  |
| C  | 1.87766700  | -4.93984400 | 0.21279600  |
| H  | 2.29415900  | -5.94320900 | 0.21207900  |
| C  | 0.47733300  | -4.76506000 | 0.28010500  |
| H  | -0.17270000 | -5.63351600 | 0.33442200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.06025500 | -3.48787900 | 0.27844100  |
| H | -1.13620600 | -3.36141500 | 0.33145800  |
| C | 0.77646600  | -2.34794800 | 0.20266500  |
| C | -2.66522600 | -1.29677800 | -1.09662900 |
| C | -2.01686300 | -1.85866700 | -2.22348700 |
| H | -0.93981100 | -1.92780200 | -2.22145200 |
| C | -2.74531200 | -2.32197300 | -3.29755300 |
| H | -2.22765600 | -2.75844900 | -4.14642700 |
| C | -4.15396700 | -2.23955800 | -3.29771000 |
| H | -4.71802300 | -2.60204100 | -4.15169100 |
| C | -4.81770500 | -1.71681500 | -2.20933800 |
| H | -5.89730800 | -1.66240900 | -2.19961900 |
| C | -4.10245900 | -1.24792300 | -1.07575000 |
| C | -4.72930200 | -0.77306700 | 0.11968800  |
| C | -6.21938100 | -0.60526400 | 0.23466500  |
| C | -8.03118400 | -0.43938300 | 1.73921900  |
| H | -8.16352200 | -0.50663100 | 2.81809700  |
| H | -8.33254300 | 0.54474600  | 1.37322400  |
| H | -8.61040700 | -1.21276100 | 1.22993400  |
| C | -3.94305700 | -0.45033300 | 1.20021700  |
| H | -4.40890300 | -0.12504800 | 2.11932900  |
| C | -2.53233700 | -0.50363300 | 1.11878300  |
| C | -1.65727600 | -0.20043800 | 2.25393800  |
| C | -2.12465900 | 0.04479100  | 3.55450300  |
| H | -3.18742200 | 0.06069000  | 3.77306300  |
| C | -1.21787400 | 0.25578700  | 4.59204100  |
| H | -1.58373100 | 0.44327200  | 5.59700200  |
| C | 0.15847600  | 0.21675800  | 4.33905800  |
| H | 0.86251300  | 0.37199200  | 5.15203500  |
| C | 0.63234000  | -0.01791800 | 3.04738600  |
| H | 1.70069700  | -0.03766300 | 2.86377000  |
| C | -0.26342100 | -0.22182400 | 1.98508500  |