**Supporting Information**

# DFT Study on C-S Bond Dissociation Enthalpies of Thiol-derived Peptide Models

Huifang Chang, Wenrui Zheng[[1]](#footnote-1)\*,Danfeng Zhu and Hongyun Xie

College of Chemistry and Chemical Engineering, Shanghai University of Engineering Science, Shanghai 201620, China

**Table S1** The 55 C-S calculated BDEs using 25 kinds of DFTs (kJ/mol)

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Entry | compounds | EXP | B3LYPa | M05-2Xb | M06-HFc | M05d | M06e | M06-2Xf | SOGGA11g | SOGGA11-Xh | M06-Li |
| 1 |  | 312.5 | 287.4 | 313.0 | 318.9 | 301.4 | 308.2 | 312.4 | 330.6 | 314.3 | 308.0 |
| 2 |  | 347.3 | 333.5 | 361.7 | 368.1 | 345.5 | 349.9 | 356.8 | 373.6 | 359.9 | 349.5 |
| 3 |  | 307.9 | 276.3 | 307.1 | 321.1 | 288.3 | 298.0 | 306.3 | 320.2 | 304.0 | 293.6 |
| 4 |  | 310.5 | 278.8 | 310.7 | 322.1 | 291.4 | 302.9 | 309.4 | 323.4 | 307.1 | 298.0 |
| 5 |  | 307.1 | 266.7 | 305.1 | 325.3 | 277.0 | 292.4 | 303.3 | 310.3 | 295.8 | 283.5 |
| 6 |  | 309.2 | 277.9 | 309.7 | 321.1 | 290.4 | 301.8 | 308.3 | 323.0 | 306.1 | 296.8 |
| 7 |  | 307.5 | 264.3 | 305.2 | 324.9 | 275.4 | 293.4 | 303.4 | 307.7 | 294.3 | 284.6 |
| 8 |  | 310 | 274.7 | 309.1 | 321.1 | 288.1 | 301.7 | 307.9 | 319.0 | 303.6 | 296.9 |
| 9 |  | 301.2 | 254.8 | 302.5 | 328.4 | 263.6 | 287.4 | 299.1 | 294.3 | 285.6 | 273.4 |
| 10 |  | 297.1 | 258.0 | 294.8 | 315.7 | 267.2 | 282.6 | 293.7 | 302.0 | 286.0 | 274.0 |
| 11 |  | 307.5 | 278.0 | 309.6 | 321.4 | 290.4 | 301.8 | 308.2 | 322.6 | 306.2 | 296.9 |
| 12 |  | 299.6 | 253.0 | 303.4 | 327.8 | 262.5 | 289.6 | 299.9 | 290.7 | 284.8 | 276.0 |
| 13 |  | 308.4 | 273.1 | 310.1 | 319.1 | 286.9 | 304.1 | 308.6 | 316.1 | 303.2 | 299.6 |
| 14 |  | 306.3 | 278.1 | 309.9 | 321.3 | 290.7 | 302.0 | 308.5 | 322.8 | 306.3 | 296.9 |
| 15 |  | 305 | 270.5 | 310.5 | 327.9 | 281.9 | 298.6 | 308.0 | 313.7 | 300.1 | 289.5 |
| 16 |  | 252.7 | 223.1 | 256.4 | 279.7 | 232.5 | 246.9 | 261.2 | 264.7 | 250.1 | 241.4 |
| 17 |  | 309.6 | 287.8 | 309.8 | 307.9 | 310.5 | 315.0 | 308.4 | 330.6 | 308.7 | 316.6 |
| 18 |  | 307.9 | 279.4 | 307.2 | 304.9 | 300.4 | 310.9 | 306.6 | 319.5 | 302.7 | 309.9 |
| 19 |  | 307.9 | 275.0 | 303.2 | 313.1 | 290.2 | 299.0 | 304.3 | 315.5 | 303.2 | 296.3 |
| 20 |  | 302.9 | 263.1 | 296.8 | 315.4 | 276.4 | 288.5 | 297.8 | 303.3 | 292.5 | 281.7 |
| 21 |  | 307.1 | 272.6 | 302.3 | 313.7 | 287.6 | 297.3 | 303.1 | 312.3 | 301.0 | 294.1 |
| 22 |  | 306.7 | 265.3 | 300.0 | 315.6 | 279.2 | 293.1 | 300.5 | 306.6 | 295.1 | 285.6 |
| 23 |  | 309.2 | 271.5 | 301.2 | 312.8 | 286.6 | 296.2 | 301.9 | 311.8 | 299.8 | 292.9 |
| 24 |  | 302.9 | 250.4 | 292.6 | 317.6 | 262.2 | 281.5 | 292.9 | 289.2 | 281.6 | 270.1 |
| 25 |  | 304.6 | 264.5 | 299.2 | 314.8 | 278.5 | 292.2 | 299.6 | 306.0 | 294.3 | 284.6 |
| 26 |  | 294.6 | 235.1 | 287.7 | 317.7 | 245.5 | 274.8 | 286.8 | 267.5 | 268.7 | 258.8 |
| 27 |  | 305 | 262.4 | 298.9 | 316.3 | 276.4 | 291.1 | 299.0 | 302.9 | 292.6 | 283.0 |
| 28 |  | 303.3 | 259.2 | 294.6 | 314.8 | 272.6 | 285.5 | 295.2 | 299.0 | 288.7 | 277.9 |
| 29 |  | 295.4 | 243.9 | 284.4 | 309.9 | 254.9 | 273.0 | 285.1 | 284.8 | 273.8 | 262.2 |
| 30 |  | 300.8 | 264.5 | 299.1 | 315.6 | 278.4 | 292.1 | 299.5 | 305.6 | 294.3 | 284.5 |
| 31 |  | 303.3 | 260.3 | 295.8 | 315.2 | 273.7 | 286.6 | 296.4 | 299.8 | 289.9 | 279.0 |
| 32 |  | 305.4 | 261.7 | 298.1 | 314.9 | 275.6 | 290.2 | 298.1 | 302.2 | 291.8 | 282.1 |
| 33 |  | 297.5 | 231.0 | 285.6 | 317.4 | 241.3 | 271.7 | 284.3 | 262.0 | 265.0 | 255.0 |
| 34 |  | 304.6 | 261.6 | 298.0 | 315.1 | 275.5 | 290.3 | 298.1 | 302.0 | 291.6 | 282.1 |
| 35 |  | 357.3 | 322.1 | 358.8 | 370.2 | 334.8 | 346.0 | 354.9 | 353.1 | 352.2 | 341.3 |
| 36 |  | 278.2 | 244.1 | 278.2 | 294.0 | 259.6 | 270.5 | 283.5 | 276.5 | 274.8 | 270.0 |
| 37 |  | 354 | 317.8 | 358.0 | 374.6 | 328.9 | 343.7 | 352.9 | 347.5 | 348.6 | 334.1 |
| 38 |  | 256.9 | 212.4 | 251.9 | 279.5 | 224.5 | 244.6 | 258.9 | 248.8 | 242.6 | 237.0 |
| 39 |  | 327.6 | 287.3 | 331.4 | 353.3 | 297.5 | 312.2 | 330.0 | 310.9 | 319.5 | 304.8 |
| 40 |  | 225.9 | 177.3 | 223.9 | 262.0 | 187.9 | 211.9 | 234.4 | 206.9 | 209.8 | 202.0 |
| 41 |  | 236.8 | 212.0 | 241.9 | 260.5 | 226.9 | 238.2 | 246.6 | 242.3 | 242.1 | 228.5 |
| 42 |  | 235.1 | 202.8 | 239.3 | 265.2 | 216.6 | 232.9 | 244.2 | 231.5 | 234.7 | 219.2 |
| 43 |  | 228 | 191.0 | 235.7 | 269.0 | 202.8 | 225.0 | 239.4 | 218.5 | 224.4 | 206.9 |
| 44 |  | 220.1 | 177.0 | 233.7 | 271.7 | 188.3 | 221.5 | 236.5 | 199.0 | 213.2 | 199.1 |
| 45 |  | 284.9 | 254.2 | 281.7 | 290.1 | 272.7 | 280.8 | 284.3 | 285.0 | 283.6 | 275.4 |
| 46 |  | 279.5 | 249.0 | 295.9 | 303.0 | 276.8 | 283.4 | 291.5 | 270.1 | 293.1 | 266.9 |
| 47 |  | 89.5 | 64.8 | 88.5 | 86.2 | 70.2 | 65.8 | 79.4 | 82.9 | 92.1 | 73.8 |
| 48 |  | 288.3 | 238.5 | 292.8 | 310.5 | 264.5 | 276.8 | 288.6 | 255.7 | 283.9 | 255.6 |
| 49 |  | 282.4 | 224.2 | 288.4 | 313.9 | 249.3 | 270.0 | 284.4 | 237.9 | 272.4 | 245.0 |
| 50 |  | 230.1 | 170.2 | 222.4 | 249.8 | 192.3 | 209.4 | 226.6 | 186.3 | 213.5 | 188.1 |
| 51 |  | 298.3 | 240.0 | 294.9 | 310.6 | 266.4 | 279.8 | 290.2 | 258.1 | 285.8 | 258.3 |
| 52 |  | 282.8 | 210.8 | 287.1 | 320.7 | 233.9 | 265.4 | 281.6 | 218.0 | 260.7 | 235.5 |
| 53 |  | 344.3 | 284.1 | 340.7 | 354.7 | 307.4 | 318.7 | 331.3 | 291.1 | 329.9 | 295.6 |
| 54 |  | 235.1 | 182.1 | 237.6 | 263.2 | 205.6 | 223.1 | 239.9 | 197.3 | 225.9 | 202.6 |
| 55 |  | 286.6 | 260.5 | 297.1 | 321.4 | 273.7 | 280.4 | 299.2 | 291.7 | 291.4 | 272.6 |

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Entry | compounds | EXP | B3P86j | B97Dk | B97D3l | BP86m | wB97n | wB97-Xn | KMLYPo | M11p |
| 1 |  | 312.5 | 307.8 | 286.8 | 296.6 | 307.0 | 311.2 | 310.1 | 320.0 | 311.3 |
| 2 |  | 347.3 | 355.0 | 331.7 | 342.4 | 352.8 | 356.3 | 354.2 | 368.6 | 351.7 |
| 3 |  | 307.9 | 296.8 | 275.8 | 285.8 | 294.3 | 302.8 | 300.8 | 312.1 | 301.5 |
| 4 |  | 310.5 | 299.9 | 279.6 | 289.1 | 296.8 | 307.1 | 304.7 | 316.5 | 305.8 |
| 5 |  | 307.1 | 288.1 | 268.8 | 278.8 | 284.1 | 297.9 | 294.6 | 306.6 | 295.4 |
| 6 |  | 309.2 | 298.9 | 279.0 | 288.4 | 295.8 | 306.3 | 304.0 | 315.5 | 304.7 |
| 7 |  | 307.5 | 286.5 | 269.3 | 279.4 | 282.4 | 298.1 | 294.4 | 305.8 | 296.7 |
| 8 |  | 310 | 296.4 | 278.7 | 288.5 | 293.4 | 305.3 | 302.5 | 313.1 | 304.8 |
| 9 |  | 301.2 | 277.4 | 260.6 | 270.5 | 272.1 | 292.0 | 287.3 | 299.0 | 289.2 |
| 10 |  | 297.1 | 279.0 | 261.2 | 271.5 | 275.7 | 288.0 | 285.4 | 296.0 | 286.3 |
| 11 |  | 307.5 | 299.0 | 279.0 | 288.4 | 295.7 | 306.3 | 304.1 | 315.6 | 304.8 |
| 12 |  | 299.6 | 276.6 | 261.6 | 271.8 | 271.0 | 293.1 | 287.8 | 299.0 | 291.6 |
| 13 |  | 308.4 | 295.9 | 279.4 | 289.0 | 292.5 | 306.4 | 302.9 | 314.0 | 308.1 |
| 14 |  | 306.3 | 299.1 | 279.2 | 288.5 | 295.8 | 306.5 | 304.2 | 315.7 | 304.9 |
| 15 |  | 305 | 292.4 | 276.0 | 285.1 | 288.0 | 303.7 | 300.2 | 311.8 | 301.5 |
| 16 |  | 252.7 | 244.9 | 222.4 | 233.6 | 240.5 | 251.9 | 250.9 | 258.5 | 252.9 |
| 17 |  | 309.6 | 310.9 | 291.9 | 301.6 | 311.4 | 302.0 | 303.0 | 320.0 | 300.0 |
| 18 |  | 307.9 | 303.4 | 284.8 | 295.4 | 301.9 | 299.3 | 299.1 | 316.1 | 294.6 |
| 19 |  | 307.9 | 295.2 | 275.5 | 285.0 | 292.1 | 301.6 | 299.6 | 311.0 | 299.8 |
| 20 |  | 302.9 | 283.6 | 264.2 | 273.8 | 278.7 | 292.9 | 290.0 | 302.6 | 289.8 |
| 21 |  | 307.1 | 292.9 | 273.9 | 283.1 | 289.2 | 299.9 | 297.9 | 309.3 | 298.9 |
| 22 |  | 306.7 | 286.4 | 267.8 | 276.8 | 280.8 | 296.8 | 293.5 | 306.5 | 293.5 |
| 23 |  | 309.2 | 291.7 | 273.0 | 282.2 | 288.0 | 298.8 | 296.7 | 308.1 | 297.6 |
| 24 |  | 302.9 | 272.0 | 256.2 | 264.9 | 265.5 | 286.1 | 281.8 | 294.7 | 282.4 |
| 25 |  | 304.6 | 285.5 | 267.3 | 276.2 | 279.9 | 296.1 | 292.8 | 305.7 | 292.7 |
| 26 |  | 294.6 | 258.4 | 247.0 | 254.7 | 250.4 | 277.9 | 271.8 | 284.8 | 275.1 |
| 27 |  | 305 | 283.6 | 265.9 | 274.5 | 277.4 | 294.8 | 291.4 | 304.5 | 292.5 |
| 28 |  | 303.3 | 279.7 | 261.5 | 270.6 | 274.1 | 289.7 | 286.7 | 299.3 | 287.5 |
| 29 |  | 295.4 | 265.0 | 250.7 | 259.7 | 259.1 | 278.1 | 274.5 | 286.1 | 274.6 |
| 30 |  | 300.8 | 285.4 | 267.3 | 276.2 | 279.8 | 296.3 | 293.1 | 305.8 | 292.5 |
| 31 |  | 303.3 | 280.9 | 262.3 | 271.5 | 275.3 | 290.7 | 287.6 | 300.5 | 288.7 |
| 32 |  | 305.4 | 282.8 | 265.5 | 274.0 | 276.6 | 294.0 | 290.6 | 303.7 | 291.5 |
| 33 |  | 297.5 | 254.5 | 244.5 | 251.6 | 245.8 | 274.7 | 268.4 | 281.5 | 273.1 |
| 34 |  | 304.6 | 282.6 | 265.2 | 273.9 | 276.4 | 293.7 | 290.2 | 303.5 | 291.6 |
| 35 |  | 357.3 | 344.9 | 326.6 | 337.6 | 338.3 | 353.2 | 348.9 | 366.4 | 345.0 |
| 36 |  | 278.2 | 305.7 | 247.6 | 256.3 | 260.7 | 277.8 | 274.3 | 284.6 | 279.9 |
| 37 |  | 354 | 339.7 | 323.3 | 335.3 | 331.7 | 351.2 | 347.2 | 362.7 | 343.6 |
| 38 |  | 256.9 | 235.6 | 217.4 | 228.3 | 228.5 | 247.7 | 245.2 | 254.0 | 248.4 |
| 39 |  | 327.6 | 350.0 | 293.3 | 306.4 | 300.8 | 325.6 | 320.5 | 334.8 | 321.0 |
| 40 |  | 225.9 | 240.1 | 185.4 | 197.6 | 190.1 | 220.1 | 216.9 | 222.2 | 224.1 |
| 41 |  | 236.8 | 230.7 | 208.3 | 219.9 | 222.5 | 246.7 | 242.3 | 253.5 | 240.8 |
| 42 |  | 235.1 | 222.4 | 201.4 | 213.6 | 212.5 | 242.0 | 236.5 | 248.5 | 235.3 |
| 43 |  | 228 | 211.7 | 192.2 | 204.6 | 200.2 | 234.9 | 228.2 | 241.0 | 227.8 |
| 44 |  | 220.1 | 199.8 | 185.5 | 197.8 | 186.8 | 229.4 | 220.7 | 233.3 | 224.1 |
| 45 |  | 284.9 | 274.3 | 251.2 | 261.4 | 268.7 | 280.1 | 277.9 | 292.8 | 276.8 |
| 46 |  | 279.5 | 273.5 | 241.7 | 253.8 | 250.0 | 296.2 | 289.9 | 323.0 | 284.6 |
| 47 |  | 89.5 | 84.8 | 65.4 | 76.4 | 76.4 | 86.9 | 83.2 | 108.2 | 78.3 |
| 48 |  | 288.3 | 263.2 | 234.4 | 246.2 | 237.8 | 290.1 | 282.4 | 316.2 | 279.5 |
| 49 |  | 282.4 | 250.5 | 227.7 | 238.0 | 223.3 | 283.1 | 273.7 | 307.8 | 274.7 |
| 50 |  | 230.1 | 195.1 | 165.5 | 178.0 | 170.5 | 222.2 | 214.8 | 244.6 | 211.9 |
| 51 |  | 298.3 | 265.1 | 238.0 | 249.1 | 239.0 | 293.0 | 285.0 | 319.3 | 282.1 |
| 52 |  | 282.8 | 238.6 | 221.7 | 230.9 | 210.1 | 276.8 | 265.6 | 299.7 | 272.2 |
| 53 |  | 344.3 | 309.4 | 279.8 | 294.9 | 281.2 | 336.5 | 328.3 | 366.2 | 320.0 |
| 54 |  | 235.1 | 207.9 | 180.6 | 193.9 | 181.4 | 235.4 | 228.6 | 257.8 | 226.8 |
| 55 |  | 286.6 | 280.6 | 255.0 | 265.9 | 272.6 | 295.5 | 291.6 | 302.1 | 295.8 |

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Entry | compounds | EXP | M11-Lq | N12-SXr | BMKs | PBE1PBEt | B3LYP-D3u | BP86-D3v | B3PW91w | CAM-B3LYPx |
| 1 |  | 312.5 | 313.5 | 321.3 | 313.9 | 305.4 | 290.2 | 310.2 | 297.8 | 292.0 |
| 2 |  | 347.3 | 353.5 | 366.9 | 358.3 | 352.6 | 337.8 | 357.7 | 344.5 | 338.0 |
| 3 |  | 307.9 | 300.1 | 309.7 | 306.8 | 295.4 | 282.6 | 301.3 | 286.5 | 282.4 |
| 4 |  | 310.5 | 304.8 | 313.3 | 310.0 | 298.8 | 286.3 | 305.1 | 289.5 | 285.8 |
| 5 |  | 307.1 | 291.3 | 300.1 | 302.3 | 287.4 | 277.6 | 296.2 | 277.0 | 274.8 |
| 6 |  | 309.2 | 303.5 | 312.4 | 308.5 | 297.9 | 285.6 | 304.3 | 288.5 | 284.9 |
| 7 |  | 307.5 | 291.2 | 298.9 | 301.4 | 286.0 | 277.4 | 296.9 | 274.9 | 273.0 |
| 8 |  | 310 | 301.6 | 310.2 | 307.4 | 295.3 | 284.4 | 304.0 | 285.6 | 281.8 |
| 9 |  | 301.2 | 281.0 | 288.4 | 296.1 | 277.2 | 270.4 | 289.6 | 265.2 | 265.3 |
| 10 |  | 297.1 | 281.4 | 290.9 | 291.9 | 278.2 | 269.3 | 288.5 | 268.1 | 265.6 |
| 11 |  | 307.5 | 303.9 | 312.4 | 308.4 | 297.9 | 285.7 | 304.3 | 288.6 | 284.9 |
| 12 |  | 299.6 | 282.2 | 288.0 | 295.7 | 276.4 | 270.9 | 291.0 | 263.9 | 264.1 |
| 13 |  | 308.4 | 303.6 | 309.8 | 307.8 | 295.1 | 285.2 | 305.7 | 284.5 | 281.2 |
| 14 |  | 306.3 | 303.9 | 312.5 | 308.7 | 298.0 | 285.9 | 304.4 | 288.7 | 285.1 |
| 15 |  | 305 | 296.4 | 305.2 | 306.7 | 292.1 | 283.7 | 302.7 | 281.3 | 279.4 |
| 16 |  | 252.7 | 246.9 | 256.7 | 255.8 | 245.1 | 232.1 | 250.8 | 235.7 | 231.4 |
| 17 |  | 309.6 | 319.8 | 325.1 | 303.7 | 308.5 | 290.1 | 313.9 | 301.2 | 287.9 |
| 18 |  | 307.9 | 313.1 | 316.3 | 300.0 | 301.6 | 286.0 | 309.3 | 292.9 | 282.3 |
| 19 |  | 307.9 | 302.5 | 308.4 | 302.6 | 294.0 | 280.7 | 298.7 | 285.1 | 281.4 |
| 20 |  | 302.9 | 288.6 | 296.4 | 294.8 | 283.4 | 272.7 | 289.5 | 273.2 | 271.1 |
| 21 |  | 307.1 | 299.6 | 306.3 | 300.8 | 291.7 | 278.8 | 296.4 | 282.7 | 279.3 |
| 22 |  | 306.7 | 292.4 | 299.5 | 297.6 | 286.4 | 276.1 | 293.0 | 275.7 | 274.2 |
| 23 |  | 309.2 | 307.6 | 305.1 | 299.6 | 290.5 | 277.8 | 295.2 | 281.5 | 278.2 |
| 24 |  | 302.9 | 276.5 | 284.0 | 287.8 | 272.5 | 265.7 | 282.8 | 260.4 | 260.7 |
| 25 |  | 304.6 | 291.5 | 298.7 | 296.6 | 285.6 | 275.5 | 292.3 | 274.9 | 273.4 |
| 26 |  | 294.6 | 263.2 | 269.6 | 279.9 | 259.3 | 256.5 | 274.6 | 245.3 | 248.1 |
| 27 |  | 305 | 289.3 | 296.9 | 295.4 | 283.6 | 273.9 | 290.2 | 272.9 | 271.7 |
| 28 |  | 303.3 | 293.4 | 292.6 | 291.5 | 279.5 | 269.5 | 285.7 | 269.2 | 267.5 |
| 29 |  | 295.4 | 268.5 | 276.8 | 279.2 | 265.4 | 259.6 | 277.0 | 253.7 | 253.6 |
| 30 |  | 300.8 | 291.6 | 298.6 | 295.9 | 285.5 | 275.6 | 292.2 | 274.8 | 273.4 |
| 31 |  | 303.3 | 285.5 | 293.9 | 293.2 | 280.7 | 270.5 | 286.8 | 270.4 | 268.7 |
| 32 |  | 305.4 | 288.5 | 296.2 | 294.7 | 282.9 | 273.5 | 289.6 | 272.1 | 271.0 |
| 33 |  | 297.5 | 258.9 | 265.8 | 277.0 | 255.4 | 253.4 | 271.1 | 241.3 | 244.4 |
| 34 |  | 304.6 | 297.8 | 295.9 | 294.8 | 282.7 | 273.1 | 289.4 | 271.9 | 270.8 |
| 35 |  | 357.3 | 342.9 | 356.9 | 351.3 | 343.8 | 335.6 | 353.7 | 332.8 | 330.8 |
| 36 |  | 278.2 | 273.2 | 319.7 | 276.0 | 267.1 | 252.3 | 269.9 | 294.6 | 254.4 |
| 37 |  | 354 | 336.5 | 351.0 | 348.7 | 338.8 | 334.3 | 350.7 | 327.7 | 327.6 |
| 38 |  | 256.9 | 241.4 | 247.3 | 248.7 | 237.1 | 227.9 | 246.3 | 225.5 | 223.4 |
| 39 |  | 327.6 | 307.4 | 361.6 | 320.9 | 311.7 | 305.2 | 321.1 | 337.8 | 300.4 |
| 40 |  | 225.9 | 205.3 | 251.5 | 218.1 | 204.5 | 198.2 | 213.9 | 229.5 | 192.6 |
| 41 |  | 236.8 | 224.9 | 243.0 | 244.2 | 231.3 | 218.8 | 230.3 | 221.4 | 222.8 |
| 42 |  | 235.1 | 216.0 | 234.1 | 240.3 | 224.0 | 215.6 | 226.9 | 212.4 | 215.4 |
| 43 |  | 228 | 203.6 | 222.5 | 234.0 | 213.9 | 208.5 | 219.6 | 200.8 | 205.6 |
| 44 |  | 220.1 | 194.2 | 210.0 | 227.8 | 202.6 | 202.6 | 215.5 | 187.2 | 194.5 |
| 45 |  | 284.9 | 283.4 | 287.9 | 279.7 | 273.6 | 258.8 | 273.9 | 264.5 | 260.8 |
| 46 |  | 279.5 | 294.3 | 289.8 | 281.9 | 277.3 | 259.1 | 262.0 | 262.1 | 268.9 |
| 47 |  | 89.5 | 77.4 | 99.0 | 75.4 | 90.0 | 71.4 | 84.0 | 77.5 | 71.6 |
| 48 |  | 288.3 | 280.1 | 279.5 | 276.9 | 268.1 | 255.0 | 257.1 | 251.4 | 260.3 |
| 49 |  | 282.4 | 266.9 | 266.7 | 269.9 | 256.3 | 249.4 | 252.3 | 237.2 | 248.8 |
| 50 |  | 230.1 | 211.8 | 209.8 | 209.5 | 200.6 | 187.0 | 190.0 | 184.3 | 192.6 |
| 51 |  | 298.3 | 282.8 | 281.9 | 278.4 | 270.3 | 258.4 | 260.2 | 253.1 | 262.6 |
| 52 |  | 282.8 | 254.2 | 254.4 | 263.6 | 244.8 | 243.7 | 247.7 | 223.8 | 238.1 |
| 53 |  | 344.3 | 318.3 | 324.6 | 319.7 | 313.5 | 305.2 | 305.2 | 296.3 | 307.4 |
| 54 |  | 235.1 | 224.7 | 222.9 | 222.1 | 214.2 | 203.3 | 206.1 | 197.0 | 205.4 |
| 55 |  | 286.6 | 276.9 | 292.8 | 294.5 | 280.7 | 265.3 | 278.1 | 271.2 | 272.2 |

**References**

aLee C, Yang W, Parr RG. Development of the Colic-Salvetti correlation-energy formula into a functional of the electron density. Phys. Rev. B: Condens.Matter Mater. Phys. 1988; 37: 785-789. doi: 10.1103/PhysRevB.37.785

b Zhao Y, Schultz NE, Truhlar DG. Design of Density Functionals by Combining the Method of Constraint Satisfaction with Parametrization for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions. J. Chem. Theory Comput. 2006; 2: 364-382. doi: 10.1021/ct0502763

c Zhao Y, Truhlar DG. Density Functional for Spectroscopy: No Long-Range Self-Interaction Error, Good Performance for Rydberg and Charge-Transfer States, and Better Performance on Average than B3LYP for Ground States. J. Phys. Chem. A. 2006; 110: 13126-13130. doi: 10.1021/jp066479k

d Zhao Y, Schultz NE, Truhlar DG. Exchange-correlation functional with broad accuracy for metallic and nonmetallic compounds, kinetics, and noncovalent interactions. J. Chem. Phys. 2005; 123: 161103-1-161103-4. doi: 10.1063/1.2126975

e Zhao Y, Truhlar DG. Density Functionals with Broad Applicability in Chemistry. Theor. Chem. Acc. 2008; 41: 157-167. doi: 10.1021/ar700111a

f Zhao Y, Truhlar DG. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. Theor. Chem. Acc. 2008; 120: 215-241. doi: 10.1007/s00214-007-0310-x

g Peverati R, Zhao Y, Truhlar DG. Generalized Gradient Approximation That Recovers the Second-Order Density-Gradient Expansion with Optimized Across-the-Board Performance. J. Phys. Chem. Lett. 2011; 2: 1991-1997. doi: 10.1021/jz200616w

h Peverati R, Truhlar DG. Communication: A global hybrid generalized gradient approximation to the exchange-correlation functional that satisfies the second-order density-gradient constraint and has broad applicability in chemistry . J. Chem. Phys. 2011; 135: 191102-1-191102-4. doi: 10.1063/1.3663871

i Zhao Y, Truhlar DG. A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. J. Chem. Phys. 2006; 125: 194101-1-194101-18. doi: 10.1063/1.2370993

j Perdew JP. Density-functional approximation for the correlation energy of the inhomogeneous electron gas. Phys. Rev. B: Condens. Matter Mater. Phys. 1986; 33: 8822-8824. doi: 10.1103/PhysRevB.33.8822

k Grimme S. Semiempirical GGA-Type Density Functional Constructed with a Long-Range Dispersion Correction. J. Comput. Chem. 2006; 27: 1787-1799. doi: 10.1002/jcc.20495

l Austin A, Petersson GA, Frisch MJ, et al. A Density Functional with Spherical Atom Dispersion Terms. J. Chem. Theory Comput. 2012; 8: 4989-5007. doi: 10.1021/ct300778e

m Hirao H. Which DFT Functional Performs Well in the Calculation of Methylcobalamin? Comparison of the B3LYP and BP86 Functionals and Evaluation of the Impact of Empirical Dispersion Correction. J. Phys. Chem. A. 2011; 115: 9308-9313. doi: 10.1021/jp2052807

n Chai JD, Head-Gordon M. Systematic Optimization of Long-Range Corrected Hybrid Density Functionals. J. Chem. Phys. 2008; 128: 084106-1-084106-15. doi: 10.1063/1.2834918

o Rzepa HS. A Double-Twist Mo 1 bius-Aromatic Conformation of [14] Annulene. Org. Lett. 2005; 7: 4637-4639. doi: 10.1021/ol0518333

p Peverati R, Truhlar DG. Improving the Accuracy of Hybrid Meta-GGA Density Functionals by Range Separation. J. Phys. Chem. Lett. 2011; 2: 2810-2817. doi: 10.1021/jz201170d

q Peverati R, Truhlar DG. M11-L: A Local Density Functional That Provides Improved Accuracy for Electronic Structure Calculations in Chemistry and Physics. J. Phys. Chem. Lett. 2012; 3: 117-124. doi: 10.1021/jz201525m

r Peverati R, Truhlar DG. Screened-exchange density functionals with broad accuracy for chemistry and solid-state physics. Phys. Chem. Chem. Phys. 2012; 14: 16187-16191. doi: 10.1039/c2cp42576a

s Boese AD, Martin JML. Development of density functionals for thermochemical kinetics. J. Chem. Phys. B. 2004; 121: 3405-3442. doi: 10.1063/1.1774975

t Ernzerhof M, Scuseria GE. Assessment of the Perdew-Burke-Ernzerhof exchange-correlation functional. J. Chem. Phys. 1999; 110: 5029-5036. doi: 10.1063/1.478401

u Grimme S, Antony J, Ehrlich S, et al. A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. J. Chem. Phys. 2010; 132: 154104-2-154104-19. doi: 10.1063/1.3382344

v Yang J, Waller MP. A Systematic Approach to Identify Cooperatively Bound Homotrimers. J. Phys. Chem. A. 2013; 117:174-182. doi: 10.1021/jp310067m

w Perdew JP, Chevary JA, Vosko SH, et al. Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation. Phys. ReV. B. 1992; 46: 6671-6687. doi: 10.1103/PhysRevB.46.6671

x Yanai T, Tew DP, Handy NC. A new hybrid exchange-correlation functional using the Coulomb-attenuating method (CAM-B3LYP). Chem. Phys. Lett. 2004; 393: 51-57. doi: 10.1016/j.cplett.2004.06.011

**Table S2** Correlations between the theoretical and experimental C-S BDEs by 25 DFT methods (kJ/mol)

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| DFT methods | MD | MAD | RMSE | DFT methods | MD | MAD | RMSE |
| B3LYP | -40.0 | 40.0 | 41.7 | M06-L | -20.2 | 20.6 | 23.4 |
| B3LYP-D3 | -27.5 | 27.5 | 28.4 | KMLYP | 6.7 | 9.2 | 12.5 |
| CAM-B3LYP | -29.0 | 29.0 | 30.2 | M11 | -8.4 | 9.4 | 11.2 |
| BP86 | -26.5 | 26.8 | 31.1 | M11-L | -12.3 | 13.7 | 15.9 |
| BP86-D3 | -12.3 | 12.9 | 16.3 | BMK | -6.1 | 8.1 | 9.9 |
| B3PW91 | -26.8 | 27.9 | 30.4 | PBE1PBE | -17.2 | 17.4 | 19.6 |
| B97D | **-**37.5 | 37.5 | 39.0 | B3P86 | -15.8 | 18.5 | 21.0 |
| B97D3 | -27.3 | 27.3 | 29.2 | N12-SX | -2.7 | 10.5 | 13.9 |
| M05-2X | -0.5 | 4.9 | 6.2 | SOGGA11 | -5.7 | 14.0 | 20.1 |
| M05 | -25.5 | 25.5 | 27.9 | SOGGA11-X | -8.1 | 9.5 | 11.7 |
| M06-2X | -0.9 | 5.3 | 6.7 | wB97 | -4.7 | 7.3 | 8.8 |
| M06 | -10.7 | 11.4 | 13.0 | wB97-X | -8.8 | 9.8 | 11.4 |
| M06-HF | 17.5 | 17.8 | 20.6 |  |  |  |   |
| **Note**: MD (mean deviation ) = Ʃ(xi-yi)/N; MAD (mean absolute deviation) = Ʃ|xi-yi|/N; RMSE (root mean square error) = [Ʃ(xi-yi)2/N]1/2 (N = 55, xi represents the C-S BDEs of DFT methods, and yi represents the experimental C-S BDEs). |

**Table S3** The Cartesian coordinates and absolute energy values (hartrees) of selected molecules and radicals

|  |  |
| --- | --- |
| Molecules: SCF energy=-1125.2582643C -0.89008300 2.43691200 -0.30295400O -0.51368800 3.47735700 0.22475000C -1.71904500 2.42444200 -1.57456300H -1.10693500 2.09716500 -2.42466400H -2.58079100 1.75170400 -1.50993400H -2.06298000 3.44179100 -1.76687700N -0.57354700 1.21491600 0.26313900H 0.13075800 1.29324600 0.99081300C -2.21312500 -0.64801400 -0.03465300O -2.69404400 -1.56963600 -0.69873400N -2.86356100 -0.07970600 1.00655400H -2.43478100 0.72371600 1.44765500C -4.19904700 -0.50524200 1.40390200H -4.21397300 -1.58373700 1.58560300H -4.47417100 0.02100600 2.32051400H -4.93430800 -0.28100500 0.62279100C -0.79266500 -0.10414400 -0.33015400H -0.70332300 -0.04859100 -1.41905500C 0.28287800 -1.11472400 0.19576800H 0.00709500 -1.39256500 1.21882000S 0.34373500 -2.67302200 -0.81520300H -0.99613100 -2.81423300 -0.94184000C 1.68627300 -0.53312200 0.22812200C 2.36391100 -0.42062000 1.44967000C 2.32922000 -0.09991300 -0.94229500C 3.65200400 0.12218300 1.50757400H 1.88567500 -0.76914600 2.36315800C 3.61216400 0.44426100 -0.88644000H 1.82875400 -0.20265100 -1.90161000C 4.27768000 0.55884400 0.33923700H 4.16234100 0.19914400 2.46408300H 4.09577800 0.77703600 -1.80117800H 5.27784000 0.98206400 0.37969400 SCF energy=-1012.1042809C 1.15114300 -2.42334700 -0.03870200O 1.58760100 -3.27320600 0.73124200C 1.16092500 -2.60867200 -1.54430400H 0.15435000 -2.52584300 -1.97131500H 1.79567800 -1.85593300 -2.02500300H 1.55551700 -3.60360700 -1.75531400N 0.60522500 -1.25983900 0.46992500H 0.76969200 -1.16655100 1.46783400C 1.47981000 0.90820600 -0.21738400O 2.30221000 0.87400700 -1.12824500N 1.66020300 1.64732800 0.91415900H 0.85043300 1.83353000 1.49012800C 2.77898500 2.57735600 1.02684100H 2.64512100 3.45216700 0.37800600H 2.86186500 2.90340100 2.06668800H 3.69922100 2.06844800 0.73364100C 0.25389700 -0.04401200 -0.25542300H 0.14969800 -0.30752800 -1.30946300C -1.10975100 0.54542300 0.20780500H -1.03998400 0.87507600 1.25338600C -2.28013000 -0.48903700 0.10630400H -2.02826700 -1.17977500 -0.71096800C -2.40264800 -1.30454900 1.40991400H -3.20337200 -2.04748000 1.31575300H -1.48479200 -1.84041000 1.65969300H -2.66319100 -0.64808300 2.25193900C -3.65387700 0.12186600 -0.21931200H -3.96828700 0.84110700 0.54960800H -3.66763100 0.62531600 -1.18942700H -4.40782500 -0.67355600 -0.24328800S -1.30554700 2.09056400 -0.82260500H -2.37608300 2.58244600 -0.16720900  SCF energy=-969.3962918C -1.90458300 -1.56099200 -0.02714400O -2.54971900 -2.36285900 0.64000500C -2.21588000 -1.30015000 -1.49127500H -2.36823100 -0.23485800 -1.69305100H -1.40124400 -1.65738000 -2.13443000H -3.12287500 -1.85211300 -1.74261800N -0.86735800 -0.85986100 0.55133400H -0.59690800 -1.19993800 1.47150200C 1.51976400 -0.52238900 0.27163600O 1.74044800 -0.97431300 1.39366900N 2.45178100 -0.45767300 -0.71130200H 2.24127700 0.12229200 -1.51334700C 3.84982300 -0.78445100 -0.45502200H 3.89975600 -1.70674900 0.12693300H 4.35895600 -0.93145600 -1.41066000H 4.35492100 0.00984000 0.10918800C 0.10686200 -0.00201000 -0.08884300H -0.04412200 -0.00470800 -1.17066900C -0.01268900 1.45960300 0.40372100H 0.14505800 1.48684700 1.48828100S -1.66480500 2.23547800 0.04831500H -2.30913700 1.72627900 1.11960100O 0.97708300 2.19354500 -0.28640200H 0.98619200 3.10839300 0.03938500 SCF energy=-1200.504245C -1.07023700 2.45078500 -0.33662100O -0.59664900 3.47033300 0.15235500C -1.97555300 2.47856800 -1.55471600H -1.44360800 2.09350800 -2.43405000H -2.87720000 1.87100600 -1.42353700H -2.25759000 3.51489100 -1.74642200N -0.79729900 1.21667500 0.22676300H -0.03637300 1.25576100 0.89863500C -2.56861900 -0.53114000 0.00235600O -3.13963600 -1.40979700 -0.64812600N -3.13412500 0.07225300 1.07369200H -2.63269500 0.84274100 1.49669000C -4.48146700 -0.25576800 1.51949600H -4.57875600 -1.33604900 1.65875500H -4.66834200 0.25101000 2.46884900H -5.23121500 0.06237800 0.78584700C -1.12434900 -0.09083000 -0.34221300H -1.06264900 -0.05777800 -1.43422400C -0.10776700 -1.16788300 0.17225700H -0.38428300 -1.41986100 1.20183100S -0.17888900 -2.73296100 -0.82849200H -1.52742900 -2.78115600 -0.93092400C 1.33114000 -0.68653200 0.17796400C 2.04182200 -0.61416600 1.38157700C 1.99097500 -0.30413100 -1.00337500C 3.36556400 -0.16555700 1.41917000H 1.56354800 -0.92084300 2.30968100C 3.30578300 0.14670000 -0.98164100H 1.47237800 -0.37255600 -1.95596500C 3.99827800 0.21859800 0.23456600H 3.89826200 -0.12097200 2.36731100H 3.81305700 0.44342200 -1.89457600O 5.29029900 0.66777000 0.19169600H 5.66955800 0.68108300 1.08446300 SCF energy=-1008.7138098C -2.30825300 1.25211000 -0.11989900O -3.17020600 1.43283700 -0.97313100C -2.52515900 1.66314500 1.32990100H -2.26611200 0.87094800 2.04085200H -1.91993400 2.54533000 1.57594000H -3.57782200 1.92323600 1.45103000N -1.10654400 0.66809800 -0.44639300H -0.93981300 0.55641400 -1.44446700C 1.31779500 0.79908700 -0.50161300O 1.22486800 0.87548000 -1.72478200N 2.48739100 0.94285700 0.16894500H 2.49787900 0.67913900 1.14754200C 3.75183600 1.11415200 -0.53486000H 3.63856100 1.87764300 -1.30793700H 4.51044400 1.43629300 0.18256800H 4.08110600 0.18495800 -1.01722300C 0.07015900 0.54867600 0.38673000H 0.05709400 1.31406400 1.17044600C 0.12910200 -0.81501100 1.13072700H -0.84061100 -0.95487200 1.62574400C 0.42592100 -2.04423700 0.25931900H 1.31274400 -1.87084600 -0.35763300H 0.63288700 -2.88686300 0.92775700S -1.01759400 -2.50468600 -0.80316400H -0.57171000 -3.75137600 -1.07407000O 1.15589500 -0.65965300 2.12833800H 1.14799500 -1.42261500 2.72697900 SCF energy=-1102.2199986C 3.29528600 0.94364800 -0.24321900O 4.20287400 1.00786000 -1.06608800C 3.52651300 1.15304100 1.24200100H 2.94706500 2.00546000 1.61836100H 3.23629300 0.26701600 1.81682200H 4.58832600 1.35492200 1.39018300N 2.00169600 0.70501900 -0.66546000H 1.94788500 0.48568800 -1.65584200C 0.80259800 -1.15038700 0.42401700O 1.28092600 -1.59085300 1.47114800N 0.33611000 -1.95260400 -0.56643600H -0.27950600 -1.55834400 -1.26874900C 0.32680700 -3.40278800 -0.41364500H -0.37326200 -3.72417700 0.36764300H 0.03510700 -3.84991500 -1.36645200H 1.32578800 -3.75054900 -0.13933500C 0.83569400 0.37566800 0.15162800H 0.98614500 0.82191500 1.13696400C -0.41182200 1.02354400 -0.48614200C -1.71492700 0.82712600 0.30800100H -0.57402000 0.66948400 -1.51074200H -0.18589800 2.09314400 -0.55834100H -1.50322900 0.81699600 1.38314200C -2.47008700 -0.44756700 -0.09580300O -2.41585300 -0.92059200 -1.22703000N -3.24245000 -0.99470300 0.88504600H -3.17201800 -0.70831200 1.85151900H -3.74560800 -1.84854500 0.67906800S -2.79320400 2.30322000 -0.04186400H -3.89324000 1.86467800 0.60827000 SCF energy= -1256.8824138C -3.22830700 1.75753300 0.39668500O -2.36796200 2.63671800 0.29722600C -4.67220100 2.08655000 0.73392100H -5.05983300 2.78133400 -0.01824100H -5.32193300 1.20669700 0.77781600H -4.70142700 2.60008700 1.70056200N -2.93990300 0.43972100 0.22007900H -3.66301700 -0.27277700 0.22337500C -1.61976200 -0.01520200 -0.17315500H -1.21406200 0.69883900 -0.89827100C -1.79996400 -1.38990000 -0.83748500O -2.82976800 -2.04992600 -0.67861700N -0.76406200 -1.81779800 -1.59829800H 0.08559400 -1.26831000 -1.60326000C -0.75032400 -3.14342000 -2.20403400H -1.68983000 -3.31515100 -2.73542500H 0.07960000 -3.19492200 -2.91260200H -0.63286800 -3.92986400 -1.44884400C -0.65361100 -0.07509600 1.05511800H -0.92343300 -0.93421700 1.67892100H -0.85410900 0.83189400 1.63610100C 1.56442700 0.96873500 0.12682700C 2.90647200 0.52146300 -0.01922000C 3.91435100 1.34105400 -0.54536000C 3.55490700 2.63044100 -0.92366000C 2.22873600 3.09769500 -0.77888300C 1.22985700 2.28376300 -0.25767700C 0.80360600 -0.11653400 0.70274200C 1.69494600 -1.15618600 0.89060400H 4.93704500 0.98727900 -0.65024800H 4.31140400 3.29377900 -1.33496300H 1.98890200 4.11441200 -1.07831300H 0.21340500 2.65266100 -0.14103500N 2.95743100 -0.77456500 0.44887800H 3.76909100 -1.37478200 0.46843700S 1.41450400 -2.79135500 1.50669300H 1.81217900 -2.58649300 2.78690000 SCF energy=-1200.5065099C 0.12291700 2.25133000 0.72341900O -0.34778700 3.25494300 0.19707100C 0.17091700 2.08127100 2.23154900H -0.51442500 1.28883300 2.55415900H 1.17462300 1.82594300 2.59038500H -0.14374800 3.02268900 2.68436600N 0.66513100 1.25174800 -0.06182100H 0.44817500 1.37590400 -1.04847500C 2.49905800 -0.41432800 -0.09650300O 2.93165100 -1.56669900 -0.17081700N 3.27754900 0.66305400 -0.35018200H 2.84111200 1.57507000 -0.33183400C 4.67460300 0.52321300 -0.73688700H 4.76695800 0.02360400 -1.70767100H 5.12027800 1.51849800 -0.79838800H 5.21579200 -0.07234500 0.00441200C 1.03946000 -0.10151300 0.33826100H 1.02681900 -0.14849100 1.43097800C 0.03713500 -1.18727100 -0.19374900H 0.30419300 -1.41249400 -1.22842600S 0.17266100 -2.77942400 0.75339500H 1.49423400 -2.91819300 0.51068400C -1.40578000 -0.70747500 -0.16805900C -1.92869900 -0.03601000 -1.28823200C -2.25946800 -0.89821600 0.92660400C -3.25329200 0.40440200 -1.32028300C -3.58484500 -0.45629200 0.91149000H -1.88200800 -1.41653300 1.80362800C -4.08346400 0.19210900 -0.21913500H -3.62959000 0.92319400 -2.20035800H -4.22197000 -0.62539800 1.77482300H -5.11283200 0.53889100 -0.24823100O -1.06838400 0.19035100 -2.34448900H -1.54403100 0.63192800 -3.06532400 SCF energy=-1180.6328368C 0.13340400 2.24550200 0.78548300O -0.35840400 3.25687000 0.29557000C 0.27198600 2.06937600 2.28849000H -0.38839600 1.27282100 2.65089700H 1.29695500 1.81844500 2.58561100H -0.01868100 3.00816100 2.76228000N 0.61741200 1.24452300 -0.03583100H 0.32597400 1.35586200 -1.00799700C 2.46474800 -0.41155900 -0.12499300O 2.89172200 -1.56638500 -0.20767800N 3.23171700 0.66606600 -0.40638000H 2.78507900 1.57378200 -0.39246900C 4.61625500 0.53257000 -0.83695300H 4.68131100 0.06275500 -1.82508000H 5.06573100 1.52713300 -0.87982100H 5.17310900 -0.08772300 -0.12866500C 1.01917900 -0.10239600 0.35164100H 1.04082000 -0.14823000 1.44388100C 0.02435500 -1.22056100 -0.13741000H 0.34494600 -1.53425500 -1.13377000S 0.15095800 -2.75083800 0.90913100H 1.47135700 -2.90815600 0.67118800C -1.41665100 -0.73526300 -0.19073700C -1.89127400 -0.07797200 -1.34972400C -2.28984700 -0.88032600 0.89509900C -3.20295600 0.41521200 -1.38151800C -3.59559200 -0.38667700 0.86078500H -1.94001000 -1.38974700 1.78870600C -4.04995800 0.26825300 -0.28452000H -3.55641000 0.92513100 -2.27562200H -4.24731400 -0.51489400 1.72038700H -5.06241900 0.66060300 -0.33083200N -1.01583600 0.17756400 -2.43829600H -0.49258800 -0.63485100 -2.75504000H -1.49629100 0.58865600 -3.23319300 SCF energy= -1584.8679399 C 0.35343900 2.43129600 0.43787000O -0.09025900 3.35303500 -0.23747100C 0.52857100 2.54609600 1.94214200H -0.16028800 1.87587400 2.46897500H 1.54815400 2.30097000 2.26145400H 0.30218500 3.57491300 2.22587100N 0.74923200 1.25594200 -0.17431900H 0.49656000 1.22817600 -1.15919600C 2.54232500 -0.45504500 0.01482000O 2.94432200 -1.60909100 0.17807500N 3.32280700 0.51037100 -0.52205000H 2.91494800 1.42331500 -0.67159200C 4.68927100 0.23825900 -0.94828100H 4.70674300 -0.50939200 -1.74837900H 5.13211200 1.16815600 -1.31135800H 5.28196900 -0.14456200 -0.11170700C 1.11759800 -0.00955100 0.45056400H 1.16413700 0.15132200 1.53120100C 0.06790800 -1.14826700 0.18713800H 0.28538100 -1.59139200 -0.78495200S 0.19581500 -2.52069200 1.43501700H 1.50092900 -2.75929800 1.17901000C -1.36102800 -0.63038900 0.18384100C -2.05748300 -0.36002000 -1.00578800C -2.04791300 -0.38714200 1.38573200C -3.36871600 0.11823000 -1.00905600C -3.35641600 0.09376300 1.40332000H -1.54432600 -0.59912400 2.32501000C -4.02130800 0.34557200 0.20170200H -3.86479100 0.31275200 -1.95420900H -3.85519200 0.26512800 2.35322100H -5.04180100 0.71828900 0.20090700Cl -1.28553100 -0.59391800 -2.58110700 SCF energy=-1313.8829009C -0.62547000 -2.44285400 -0.61050100O -0.18899400 -3.01257700 -1.60538800C -0.95433300 -3.19621300 0.66737400H -0.26801100 -2.91713500 1.47525700H -1.97637500 -3.00152000 1.01237100H -0.84091800 -4.26218100 0.46487400N -0.86888800 -1.08424000 -0.64394200H -0.52467000 -0.63558800 -1.48944200C -2.56191300 0.52043600 0.21442400O -2.88744100 1.53560400 0.83343000N -3.37636400 -0.06420600 -0.69419800H -3.01298800 -0.84910900 -1.21794100C -4.69019700 0.48119000 -1.00768500H -4.60692700 1.46053300 -1.49235000H -5.20429000 -0.21131200 -1.67780800H -5.27664000 0.60414200 -0.09253500C -1.20481500 -0.19653200 0.46243300H -1.34196400 -0.80892500 1.35794800C -0.07633800 0.84977200 0.77230900H -0.22321000 1.70657400 0.12029000S -0.19571200 1.50330000 2.51296100H -1.45001300 1.97753200 2.34757600C 1.32407300 0.28296400 0.57023600C 2.13584500 0.60134500 -0.54533400C 1.86858300 -0.56197400 1.54973100C 3.45126100 0.10979900 -0.62461200C 3.16160300 -1.07419300 1.44641900H 1.27382400 -0.80177100 2.42659600C 3.96399200 -0.73135000 0.35667000H 4.05561400 0.39439000 -1.47970500H 3.54410300 -1.72844500 2.22554000H 4.97720400 -1.11358100 0.27213900C 1.72369600 1.43558700 -1.71243700O 2.47861500 2.10212800 -2.38912800O 0.39357500 1.34825000 -2.02846100H 0.26146000 1.91762700 -2.81098800 SCF energy=-1462.4052357C 1.05332300 2.36647900 -1.02397200O 0.62000000 2.81934500 -2.07781800C 1.65229500 3.25842300 0.05009600H 1.01435100 3.28197100 0.94169900H 2.64943600 2.92472300 0.35933600H 1.72112500 4.26872600 -0.35570300N 1.03527300 1.00368000 -0.79785100H 0.53309800 0.49039000 -1.51704400C 2.63628900 -0.58027500 0.27977800O 2.99284500 -1.36970600 1.15811000N 3.34476200 -0.39838500 -0.85655400H 2.98195100 0.24603500 -1.54585300C 4.57347200 -1.13677500 -1.11814700H 4.37830300 -2.21331900 -1.16277700H 4.98281200 -0.80251900 -2.07375600H 5.30576100 -0.95584900 -0.32513400C 1.35490700 0.28776300 0.43195100H 1.57554900 1.02508500 1.20792400C 0.15070300 -0.58708600 0.93605200H 0.17519800 -1.53356800 0.39981500S 0.28923600 -1.00601400 2.74390100H 1.53381000 -1.52265000 2.63028500C -1.19246200 0.10417300 0.72867000C -2.14617300 -0.32661100 -0.21973300C -1.50842300 1.22987200 1.50288200C -3.36115900 0.35412900 -0.36987000C -2.71673900 1.90959800 1.35142700H -0.79826100 1.56541700 2.25322800C -3.64936400 1.47107900 0.41180400H -4.08066500 0.00762000 -1.10280700H -2.92786800 2.77734800 1.97058700H -4.59450200 1.99094300 0.28526000C -1.89304600 -1.52628100 -1.10178100F -2.88919100 -1.74778200 -1.98558000F -1.73507800 -2.67451700 -0.39617600F -0.74935500 -1.38161600 -1.84979100 SCF energy=-1217.5235722C -0.25610300 -2.40750300 0.46689400O 0.16636300 -3.34560000 -0.19873900C -0.35562300 -2.47298900 1.98116200H 0.33958900 -1.76934800 2.45301600H -1.36520900 -2.24093600 2.33965000H -0.09113400 -3.48587600 2.28813700N -0.69777000 -1.25773300 -0.16312800H -0.52234500 -1.27033900 -1.16515700C -2.50300700 0.43935500 0.05019400O -2.91331300 1.59206800 0.20132300N -3.29248900 -0.54944000 -0.42543100H -2.88128800 -1.46138700 -0.57093200C -4.67703100 -0.30225800 -0.80809400H -4.73089600 0.41980000 -1.62958000H -5.12349400 -1.24684700 -1.12569800H -5.24096000 0.10059900 0.03872700C -1.05402100 0.02323200 0.43594500H -1.04938400 -0.10078500 1.52228400C -0.02646300 1.15808400 0.08274000H -0.27096900 1.53322700 -0.91395600S -0.13431800 2.60325700 1.24571600H -1.45447200 2.79832000 1.03080800C 1.41041800 0.65957500 0.08121600C 2.06913500 0.35519000 -1.13322800C 2.12649000 0.47609000 1.27056300C 3.39688200 -0.10790100 -1.14305100C 3.44431600 0.01442400 1.26232000H 1.65066900 0.71733000 2.21677300C 4.08434000 -0.27675100 0.05495900H 3.87209000 -0.33423300 -2.09244900H 3.97313500 -0.11253400 2.20316200H 5.10998300 -0.63373600 0.04636800C 1.37789800 0.48034400 -2.38568200N 0.80254400 0.55424900 -3.39557000 SCF energy=-1356.3663279C 2.21592700 1.21623000 -1.92799700O 1.83837900 1.47614100 -3.06574800C 3.56028600 1.67584700 -1.39318400H 3.42485600 2.47696500 -0.65554400H 4.11742700 0.86798700 -0.90640700H 4.14224800 2.06816600 -2.22845400N 1.41739500 0.47123700 -1.08311900H 0.47977300 0.33181400 -1.44728300C 2.48745500 -1.09775700 0.54129700O 3.02950300 -1.33918100 1.62316700N 2.56062800 -1.93971300 -0.51447300H 2.14774100 -1.63992100 -1.38784300C 3.29592300 -3.19525600 -0.44674200H 2.92371100 -3.81070800 0.37780000H 3.15853500 -3.73031400 -1.38882100H 4.36445800 -3.01657400 -0.28332600C 1.64836700 0.18928400 0.33276200H 2.21655300 1.00487800 0.78829200C 0.27288600 0.06630200 1.07232700H -0.16756800 -0.88814300 0.77856500S 0.44186300 0.05975500 2.92295900H 1.51105500 -0.76804600 2.97103900C -0.68968000 1.19029400 0.70927600C -1.92517200 0.93765700 0.06893500C -0.32263000 2.51820200 0.98191300C -2.73136600 2.03174200 -0.29959400C -1.13540100 3.58869900 0.61767200H 0.61510000 2.71063400 1.49678100C -2.34708200 3.34360500 -0.03383100H -3.68397300 1.83612300 -0.78493300H -0.82551700 4.60616300 0.84080400H -2.99298600 4.16805800 -0.32419300C -2.42369200 -0.43701600 -0.24436700C -2.71996500 -0.79365300 -1.57141900C -2.65327700 -1.38288500 0.77042000C -3.22021900 -2.06215600 -1.87791800H -2.55014200 -0.07305000 -2.36832000C -3.15565500 -2.64962900 0.46425200H -2.44629700 -1.11940100 1.80477800C -3.43918800 -2.99479000 -0.86071600H -3.43784000 -2.31952000 -2.91152800H -3.33066200 -3.36501600 1.26389400H -3.83060400 -3.98083700 -1.09735700 SCF energy=-1087.349875C 2.61917100 -0.34085200 -0.06444800O 2.94698100 0.40937600 0.84728000C 3.66260200 -1.13375900 -0.84479200H 4.15044700 -1.83888200 -0.16291300H 3.25698900 -1.68804200 -1.69693900H 4.43055700 -0.43990000 -1.20021300N 1.32629500 -0.56312100 -0.47368500H 1.16630400 -1.30318900 -1.15372600C -0.97603600 -1.17045700 -0.40575600O -0.68294100 -1.97552400 -1.29609000N -2.16177000 -1.17378000 0.22855800H -2.36537000 -0.38922300 0.83906900C -3.23412900 -2.08150400 -0.15628200H -2.85046500 -3.10308000 -0.21892000H -4.01872200 -2.03472400 0.60216800H -3.65781100 -1.81532900 -1.13255800C 0.06421700 -0.07957500 0.08284900C -0.30266400 1.36179700 -0.46437200C 0.87009400 2.34269700 -0.30330100H 1.23372800 2.37081800 0.72453600H 1.70397000 2.06003300 -0.95383500H 0.53744200 3.34534100 -0.59119400C -0.72671600 1.29441900 -1.93901300H -1.63830600 0.70880900 -2.09226500H -0.89617900 2.30534600 -2.32507400H 0.07290800 0.84040600 -2.53573200S -1.72808800 2.02221500 0.58833300H -2.40658200 2.57613200 -0.44008600O 0.04595800 0.03441200 1.48526600C 0.46098000 -1.09721900 2.25166700H 0.20147400 -0.85784400 3.28512300H -0.06963000 -2.00889900 1.94716700H 1.54188400 -1.24430700 2.17699100 SCF energy= -1106.7726416C 2.68134300 -0.22951700 -0.18168600O 3.02400700 0.55148100 0.69881700C 3.72363600 -1.02830100 -0.96208900H 4.20227300 -1.73866800 -0.27843700H 3.31795100 -1.58183100 -1.81519500H 4.49901300 -0.34117400 -1.31378400N 1.38887200 -0.48007900 -0.57208500H 1.24915300 -1.19869800 -1.27814000C -0.88808100 -1.17884300 -0.54850200O -0.53262000 -1.96481100 -1.43344200N -2.10818100 -1.25955500 0.02438100H -2.40808200 -0.49712900 0.61926500C -3.09861100 -2.22593900 -0.43448100H -2.66948700 -3.23127200 -0.42622700H -3.95504900 -2.19295000 0.24273600H -3.43406000 -2.00765500 -1.45575700C 0.10903500 -0.08446500 0.04409000C -0.27631600 1.36845900 -0.50528400C 0.68191500 2.45995000 0.00987300H 0.68730100 2.55256700 1.09690600H 1.70712000 2.23271400 -0.28590900H 0.38850200 3.42281900 -0.42022800C -0.22975900 1.36788100 -2.04706100H -0.89056400 0.61503200 -2.48993800H -0.52901900 2.35245400 -2.41869600H 0.78754600 1.16690000 -2.39467200S -2.01859500 1.93417700 -0.02276100H -2.64309300 1.54439000 -1.15429400N 0.23776200 -0.20314100 1.49603900C -0.59562900 0.50733900 2.44927400H -1.61322800 0.08777100 2.56955500H -0.10203500 0.43993100 3.42637300H -0.69173800 1.56582800 2.21505600C 0.54583300 -1.54574700 1.97869200H 1.20917300 -2.06463100 1.28460200H 1.06321100 -1.46543200 2.94126100H -0.35783800 -2.16663800 2.12140100 SCF energy=-1161.4230171C 2.59835100 -0.26008600 -0.19600000O 2.80538700 0.48716400 0.75591800C 3.72359600 -0.98842000 -0.91003400H 4.07317800 -1.80611800 -0.26893800H 3.42746600 -1.40444600 -1.87800900H 4.55864100 -0.29673400 -1.05058900N 1.34417500 -0.49926100 -0.69311000H 1.20923100 -1.28400600 -1.32878700C -0.90340100 -1.26741000 -0.41931300O -0.57321500 -2.12612400 -1.23869800N -2.08820500 -1.27505600 0.21890700H -2.36250000 -0.43220600 0.71762500C -3.09622600 -2.28827400 -0.06906400H -2.64979400 -3.28325200 0.00174000H -3.89725500 -2.19684800 0.66769600H -3.51315800 -2.16962700 -1.07652700C 0.09789200 -0.09770000 -0.04942100C -0.39169800 1.30773500 -0.61637200C 0.68061300 2.39700200 -0.43068700H 0.93582800 2.54407600 0.61941400H 1.59375100 2.13546300 -0.97279300H 0.29787300 3.34009700 -0.83307800C -0.71697200 1.16643100 -2.11361400H -1.53392700 0.46351700 -2.30822900H -0.99453700 2.14150900 -2.52696100H 0.16811500 0.81363200 -2.65394200S -1.93855700 1.91373300 0.28933700H -2.71468100 1.99893800 -0.81426500C 0.26243100 -0.09099200 1.48883700O -0.10204400 0.79398700 2.22932700O 0.77290100 -1.26116100 1.92780400H 0.87514000 -1.18415300 2.89486500 SCF energy=-1200.7302312C -2.46036200 -0.42157700 -0.62957300O -2.74752800 -0.59085900 0.55270000C -3.52555600 -0.34824900 -1.71060500H -4.07710700 0.59179400 -1.59486600H -3.12176000 -0.39649000 -2.72656700H -4.23483200 -1.16763400 -1.56276600N -1.17217400 -0.29207900 -1.07514900H -1.01701300 0.06921300 -2.01506900C 0.93230800 0.83963500 -1.07490900O 0.64239000 1.10952200 -2.24195100N 2.01434500 1.34336400 -0.45128000H 2.29559300 0.91293900 0.42645500C 2.95625100 2.20726700 -1.15197500H 2.41576800 3.02211000 -1.64009000H 3.65404500 2.62191100 -0.42106600H 3.51660800 1.65921800 -1.91933800C 0.00038400 -0.11315000 -0.22414800C 0.69055700 -1.51952900 0.06344500C -0.30258000 -2.51665500 0.68840800H -0.70961600 -2.15023000 1.63150800H -1.13502800 -2.70930900 0.00524100H 0.21629000 -3.46238200 0.87446700C 1.23091400 -2.10054200 -1.25473600H 2.01061500 -1.47767700 -1.70548300H 1.64463700 -3.09906800 -1.07946400H 0.41492400 -2.19832800 -1.97888100S 2.12496800 -1.33996500 1.28462600H 3.05621100 -1.89620800 0.47681800C -0.38119400 0.63502900 1.07907800O -0.04971700 0.29456100 2.19388600O -1.04726100 1.76455300 0.79900400C -1.52093400 2.51160800 1.93681400H -0.68307400 2.81010400 2.57217900H -2.02065200 3.38524500 1.51804900H -2.22210400 1.90001200 2.50994900 SCF energy=-1065.0569625C 2.61177300 -0.54244900 0.07659200O 2.87460900 0.16728500 1.03906700C 3.67070600 -1.37311700 -0.63023300H 3.98298100 -2.18193200 0.03988600H 3.33165200 -1.81047600 -1.57459600H 4.54495100 -0.74272400 -0.81555800N 1.34639200 -0.65829700 -0.44614700H 1.17187600 -1.30199800 -1.21265200C -0.98799600 -1.15587200 -0.34094500O -0.85176900 -1.73125900 -1.42174300N -2.02472200 -1.36687300 0.48546400H -2.07486400 -0.84896800 1.35383300C -3.09642000 -2.29566400 0.14567800H -2.67752300 -3.26560500 -0.13647800H -3.73764700 -2.41643100 1.02073100H -3.69377200 -1.92100100 -0.69310000C 0.11020700 -0.11183700 0.10968800C -0.20606800 1.34823900 -0.47901200C 0.81668400 2.37015500 0.04884500H 0.80064000 2.44626400 1.13998900H 1.82957000 2.08518300 -0.24439700H 0.59135500 3.35425300 -0.37368400C -0.18792500 1.33239900 -2.01485700H -0.91994700 0.63948400 -2.43893100H -0.40545600 2.33902000 -2.38376200H 0.80328800 1.04158200 -2.37947500S -1.86190700 1.96456200 0.12770600H -2.62775400 1.29858300 -0.76405500C 0.14765300 -0.06753000 1.58687100N 0.02358200 -0.06945300 2.74134000 SCF energy=-1203.895889C 1.42306900 2.23641400 -0.33637900O 2.11414200 1.93092000 0.62957700C 1.82457300 3.37205700 -1.26971600H 2.72819100 3.07245300 -1.81274600H 1.05172800 3.64302600 -1.99612500H 2.07902000 4.24978900 -0.66831400N 0.24563100 1.61788600 -0.66974900H -0.19256300 1.86431700 -1.55517200C -1.19564600 -0.16335400 -1.32571800O -1.37395000 0.53022100 -2.33303200N -1.73606900 -1.38746600 -1.19634500H -1.62363000 -1.87356800 -0.31418200C -2.58804500 -1.96083900 -2.22886800H -2.05323700 -2.00893300 -3.18247800H -2.86886100 -2.97065000 -1.92186900H -3.49359800 -1.36123200 -2.37617100C -0.29135600 0.35836400 -0.13227100C -1.22342600 0.69849900 1.12449800C -0.50056800 1.55178300 2.18583300H 0.42667900 1.10458300 2.54232300H -0.24782600 2.53140900 1.77078600H -1.17092400 1.70102300 3.03822900C -2.46353600 1.48466600 0.65336100H -3.10810600 0.90662700 -0.01584900H -3.05569500 1.79588500 1.52058800H -2.14822200 2.38928900 0.12295600S -1.83177200 -0.88673400 1.97426100H -3.14266500 -0.56508100 1.96235600C 0.85346700 -0.66372400 0.06816100C 1.56955700 -1.04669800 -1.07989200C 1.22980100 -1.22969000 1.29067800C 2.61862500 -1.96091200 -1.01080600H 1.30605400 -0.61827400 -2.04426700C 2.27983800 -2.15133800 1.36461500H 0.73456100 -0.95386000 2.21307700C 2.97937600 -2.52273100 0.21760800H 3.15359600 -2.23406800 -1.91698500H 2.55264400 -2.56728800 2.33110800H 3.79838100 -3.23474000 0.27824800 SCF energy=-1012.0986982C 2.74965600 0.72035400 -0.07367600O 3.81075500 0.35214100 -0.57780400C 2.67936800 2.03277600 0.68519300H 1.83799200 2.65907700 0.38039900H 2.59274100 1.85183000 1.76155900H 3.61342200 2.56402000 0.49479100N 1.64565200 -0.09774200 -0.20734300H 1.92175500 -0.94493600 -0.69322400C -0.13974700 -1.56937500 0.48277600O -0.50488200 -1.98274200 1.57666000N 0.00625700 -2.41630400 -0.58147700H 0.14045600 -2.04221800 -1.51029100C -0.29936400 -3.83792900 -0.45758600H -1.36995400 -4.00618600 -0.29100500H 0.00965900 -4.34228000 -1.37617200H 0.24769700 -4.26143900 0.38837700C 0.22653100 -0.06339300 0.23214800C -0.67036900 0.49960600 -0.93862400H -0.41480600 -0.11278000 -1.81650600C -0.33893100 1.94356000 -1.34431900H -0.53371000 2.66124500 -0.54115100H 0.70831700 2.03327500 -1.64627800H -0.95806700 2.24065400 -2.19845600C -2.19186700 0.27737000 -0.75390500H -2.39067200 -0.69842400 -0.30202600H -2.65649900 0.29140200 -1.74470600S -3.04170700 1.57456600 0.26894900H -4.24963700 0.97306400 0.25164000C 0.02701900 0.67215200 1.56233200H 0.74334200 0.31174700 2.30462400H 0.13400200 1.75165800 1.45422900H -0.97283700 0.46964800 1.94587000 SCF energy=-1028.1591438C 2.49576900 1.20638200 0.06129900O 3.31036700 1.90714600 -0.53381200C 2.83048700 0.54798800 1.38565100H 2.36563400 1.10596600 2.20701800H 2.48353000 -0.48626500 1.45954300H 3.91403300 0.58330700 1.51215900N 1.23775200 1.02143200 -0.48223100H 1.10467300 1.58781100 -1.31257400C 0.38445100 -1.19977100 0.21940600O 0.09694500 -1.81313800 1.24405500N 0.98096000 -1.78752700 -0.84904400H 1.36284800 -1.18391500 -1.56529500C 1.39020400 -3.18627200 -0.82227200H 0.57669500 -3.79566200 -0.42228300H 1.61494400 -3.50637200 -1.84248600H 2.27528500 -3.33907800 -0.19204300C 0.05030000 0.32102800 0.04927700C -1.08558400 0.48441100 -1.02617900H -0.68742000 0.08832100 -1.97301600C -1.48146000 1.95359600 -1.25165400H -1.82277200 2.41755600 -0.32280000H -0.66505900 2.55711000 -1.66449400H -2.31039500 2.00487300 -1.96676500C -2.31820700 -0.39204500 -0.72024000H -2.01898100 -1.42958900 -0.54925400H -2.95734800 -0.37408300 -1.60740000S -3.36084500 0.16396700 0.71378500H -4.52488700 -0.26279800 0.16945800N -0.42763000 0.81110400 1.32806200H -0.20571900 0.17408900 2.08839300H -0.12336400 1.75622500 1.53009600 SCF energy=-1072.0492052C 2.61714400 0.95857300 0.01995300O 3.77386700 0.72169000 -0.31022300C 2.24505000 2.23340400 0.74433900H 1.28763100 2.65178300 0.43443000H 2.17499300 2.02313800 1.81737300H 3.04635700 2.95557100 0.57706500N 1.65259200 -0.01096800 -0.24477100H 2.09502700 -0.87832700 -0.52992600C -0.05182500 -1.60778400 0.43485300O -0.47509900 -1.94038000 1.52875000N 0.23265900 -2.50292400 -0.55766800H 0.41902100 -2.17252300 -1.49485100C -0.00860000 -3.93168000 -0.37069100H -1.08083200 -4.15836500 -0.34062700H 0.45564700 -4.47497500 -1.19679500H 0.43765800 -4.25632300 0.57198000C 0.23877400 -0.10593800 0.09220900C -0.71980800 0.40626900 -1.02367000H -0.52644900 -0.25893900 -1.87967500C -0.42981900 1.83187200 -1.50484400H -0.62092400 2.56494700 -0.71687800H 0.60259900 1.93645600 -1.85052300H -1.08632600 2.07227600 -2.35005900C -2.21447700 0.18924800 -0.67541200H -2.36588200 -0.78519400 -0.20275000H -2.79275400 0.18125500 -1.60387700S -3.01821900 1.39507500 0.47082800H -3.38522200 2.28861600 -0.47308100F -0.00161900 0.61026600 1.25259700 SCF energy=-1086.1159996C -2.81923300 0.56677300 0.16911700O -3.90264400 0.15473500 0.57272000C -2.69752900 1.94437300 -0.45323400H -1.70369900 2.38802900 -0.41050100H -3.00102300 1.87916500 -1.50528100H -3.41052400 2.59945700 0.05291800N -1.72389100 -0.27796500 0.25200400H -2.01599700 -1.19422200 0.57716000C 0.18310100 -1.59217100 -0.46564800O 0.65210800 -1.85119400 -1.56878600N 0.01998400 -2.53751700 0.50242100H -0.18454000 -2.24620000 1.44932200C 0.46363700 -3.91378900 0.29284900H 1.55752100 -3.98878600 0.29044000H 0.05626000 -4.53695200 1.09211100H 0.09292500 -4.27161000 -0.66999800C -0.29917800 -0.14940000 -0.11775400C 0.55973900 0.43266900 1.06551200H 0.27238000 -0.20463200 1.91682400C 0.19797800 1.86542600 1.48201700H 0.41901400 2.58913700 0.69511900H -0.85709600 1.94066300 1.76126100H 0.79028300 2.14531800 2.36079300C 2.09044600 0.21776400 0.94942100H 2.31237900 -0.78655600 0.57692700H 2.49116700 0.28629900 1.96508400S 3.03510200 1.44525400 -0.07410200H 4.19451400 1.24980700 0.59432900C -0.19195300 0.59700200 -1.46559300O 0.53814500 1.53635800 -1.67101900H -0.87076100 0.20431000 -2.24528200 SCF energy=-1177.3156804C 2.35821700 1.43830300 -0.41924600O 3.53476900 1.41678300 -0.74995900C 1.70373200 2.72438500 0.03492400H 1.83900900 3.47762800 -0.74722900H 0.64787900 2.65608700 0.28704400H 2.25195900 3.06455100 0.91935100N 1.66089800 0.22199900 -0.44472900H 2.34067400 -0.53188200 -0.45352100C 0.35694900 -1.69659200 0.30023800O -0.12963900 -2.16024400 1.31901100N 0.93410100 -2.45947400 -0.66680700H 1.19883800 -2.03976200 -1.54818800C 0.96750800 -3.91631000 -0.55181300H -0.03147900 -4.34977600 -0.67450500H 1.63369800 -4.30925800 -1.32264000H 1.34686600 -4.19650100 0.43340700C 0.34194700 -0.15474300 0.00471200C -0.79854300 0.13418200 -1.04137000H -0.45889600 -0.49083100 -1.87966600C -0.86278300 1.55901500 -1.60207700H -1.20652000 2.28280700 -0.86080300H 0.10130000 1.87357000 -2.01045800H -1.58589000 1.57635900 -2.42525700C -2.20020200 -0.44265100 -0.66255100H -2.11333500 -1.20804100 0.10925800H -2.61709300 -0.93055600 -1.54738300S -3.49721100 0.72912600 -0.05440100H -4.18569400 0.80262900 -1.21461300N 0.07220000 0.47297200 1.41828200O -1.07128000 0.82526600 1.67104300O 1.03149100 0.56006600 2.17009400 SCF energy=-1498.5283044C 0.84295400 1.39795400 2.23186400O 1.26714800 2.42509600 2.74861000C 1.25604600 0.04107000 2.76439400H 0.99403700 -0.00405600 3.82601700H 0.82120300 -0.82103700 2.26079300H 2.34663200 -0.02126600 2.69574200N -0.01484100 1.51952400 1.14497200H -0.00368400 2.48024400 0.81849600C -0.88120600 1.30525900 -1.13088800O -0.54388500 0.83848900 -2.21147900N -1.53278500 2.49293800 -1.00939600H -1.94139900 2.75000000 -0.12037700C -1.91375100 3.26560900 -2.19021800H -2.73561300 2.78677300 -2.73493600H -2.22014800 4.26328000 -1.86845000H -1.05657600 3.34812100 -2.86165200C -0.58630300 0.54299600 0.20785000C -1.95805000 -0.05208200 0.72811200H -2.57881600 0.84903600 0.82690200C -1.90935800 -0.66864600 2.13017300H -1.31997300 -1.58739900 2.16072600H -1.52135000 0.04471100 2.86219700H -2.92763700 -0.93041100 2.43924800C -2.69645000 -0.94560600 -0.32140400H -2.29117400 -0.78958000 -1.32253000H -3.74568600 -0.64214600 -0.36056700S -2.69146200 -2.78086200 -0.08371800H -3.89766700 -2.85695200 0.52024000C 0.42656000 -0.54629300 -0.20196800O 0.20024400 -1.71378700 -0.33075700O 1.67276200 0.02916400 -0.41063900C 2.71699600 -0.74862300 -0.86347500F 3.04923700 -1.70235300 0.02349700F 2.45404500 -1.32834100 -2.03775800F 3.76559100 0.07021700 -1.01283900 SCF energy= -1332.1118014 C -2.94205200 2.17517300 0.33269400O -2.03859500 3.00620600 0.24378100C -4.35748100 2.56767900 0.71967200H -4.73342400 3.28658400 -0.01560500H -5.04964400 1.72101700 0.77311700H -4.33266700 3.07198300 1.69090700N -2.73708300 0.84794900 0.07758700H -3.48090500 0.18665300 0.25416000C -1.42468500 0.33066400 -0.30181100H -0.94139600 1.10137600 -0.90352900C -1.61137800 -0.87913200 -1.24338800O -1.43670400 -0.77135200 -2.45376900N -2.05074600 -2.02550100 -0.65238200H -1.95027800 -2.08556000 0.35715300C -2.24897500 -3.24146700 -1.42935700H -1.29885800 -3.65327400 -1.79250600H -2.74540500 -3.98306600 -0.79838900H -2.87731900 -3.02634300 -2.29753400C -0.53231300 0.09784900 0.94892000H -0.54481300 1.05161700 1.49294500C 1.81563000 0.82438500 0.14091200C 3.06367500 0.20082200 -0.11569800C 4.18302300 0.91657000 -0.55694800C 4.03039300 2.28706800 -0.74234700C 2.79820700 2.92887100 -0.48972600C 1.68894500 2.21463100 -0.05109400C 0.89817800 -0.20279900 0.58553500C 1.61127700 -1.38749300 0.58225900H 5.13227900 0.42344700 -0.75055200H 4.87623800 2.87440500 -1.08985000H 2.71528800 4.00083100 -0.64655200H 0.74359300 2.72078900 0.12812800N 2.91328200 -1.14197300 0.16650600H 3.58569000 -1.86853400 -0.03218900S 1.12033100 -3.05011200 0.96081000H 1.98080800 -3.25358100 1.98934000O -1.17299200 -0.89495400 1.76576000H -0.53098300 -1.24601600 2.40210000  SCF energy=-1371.4176183C -2.74246500 2.39333500 0.10066300O -1.76922100 3.14551600 0.05038100C -4.13449800 2.90544600 0.42967700H -4.42258700 3.64203400 -0.32754100H -4.89559300 2.11918800 0.46552000H -4.10462200 3.42063700 1.39503100N -2.63872900 1.05326000 -0.14347900H -3.44580100 0.45818700 -0.01615200C -1.36718700 0.42568900 -0.49709400H -0.82071100 1.13276800 -1.12355200C -1.65188600 -0.79702000 -1.39622300O -1.47175600 -0.74438700 -2.60927500N -2.19108300 -1.87898000 -0.76576200H -2.05318600 -1.93168900 0.23953100C -2.46456500 -3.10762100 -1.49892300H -1.54058600 -3.62299900 -1.79059400H -3.06068500 -3.76935000 -0.86522800H -3.02503700 -2.87377700 -2.40711000C -0.49489900 0.17444400 0.76422000H -0.45446000 1.14650900 1.27657000C 1.92781800 0.76093700 0.06431200C 3.13023100 0.05738000 -0.21112300C 4.31172000 0.71038900 -0.58683600C 4.26958300 2.09665700 -0.68661700C 3.08317400 2.81678200 -0.42018000C 1.91263500 2.16636800 -0.04880900C 0.92270700 -0.21488000 0.41913800C 1.53760900 -1.45202000 0.34566100H 5.22372800 0.15698000 -0.79613300H 5.16631600 2.63652200 -0.97941100H 3.08636700 3.89919100 -0.51546100H 1.00189400 2.73170400 0.13284100N 2.86551500 -1.28117100 -0.02734900H 3.49659800 -2.04848400 -0.20825700S 0.93053800 -3.10130900 0.58078000H 1.37266100 -3.28626200 1.84957600O -1.18096600 -0.74809900 1.61246400C -0.77829000 -0.69934900 2.97398700H -0.96944400 0.29582200 3.40108800H -1.37569100 -1.44353600 3.50645800H 0.28772800 -0.93772300 3.08679800 SCF energy=-1716.4786014C -2.38941200 2.67455700 -0.10711200O -1.30670600 3.25569900 -0.17049400C -3.69067200 3.42098700 0.12601200H -3.81567400 4.16333900 -0.66882300H -4.57211000 2.77219400 0.15021400H -3.62097400 3.96267600 1.07478900N -2.48913800 1.31654400 -0.23741800H -3.39816200 0.87645300 -0.19550300C -1.33023700 0.47856900 -0.53400300H -0.73835400 0.98032500 -1.30614600C -1.79704500 -0.84138300 -1.18113000O -1.40135300 -1.16849700 -2.29377800N -2.73773600 -1.54843000 -0.48422000H -2.74815800 -1.41394400 0.52161300C -3.20099000 -2.83874500 -0.98410400H -2.40861300 -3.59585400 -0.93974900H -4.05185800 -3.16297700 -0.37953200H -3.51680500 -2.73101200 -2.02394200C -0.36100200 0.38119900 0.67724500H -0.19756000 1.41140000 0.98998900C 2.13643100 0.56943100 0.09390700C 3.20862700 -0.32336200 -0.17168200C 4.49574900 0.12425300 -0.49731900C 4.69738400 1.49850700 -0.55430100C 3.64350100 2.40523500 -0.30030000C 2.36732800 1.95772100 0.01812100C 0.96797000 -0.23253900 0.37819400C 1.36598300 -1.55416700 0.28248500H 5.30382100 -0.57390800 -0.70046700H 5.68278600 1.88260600 -0.80433300H 3.83516700 3.47294300 -0.36327000H 1.56238500 2.66819900 0.18742200N 2.71055800 -1.60094700 -0.04306800H 3.22435600 -2.46240200 -0.16232300S 0.48759800 -3.08216800 0.47037400H 0.51281400 -3.13355100 1.82341000Cl -1.19162700 -0.35242200 2.16833500 SCF energy=-1370.2083816C -2.51492000 2.62507800 0.05653400O -1.44494500 3.21796000 0.17371000C -3.84933400 3.34077400 0.16943100H -3.92865300 4.06492600 -0.64850100H -4.71360000 2.66959300 0.13419800H -3.87047500 3.90270400 1.10814500N -2.57203300 1.27233400 -0.16910900H -3.46799500 0.86423500 -0.40391000C -1.36756800 0.49463100 -0.49129600H -0.77594500 1.05252800 -1.22103500C -1.76749800 -0.81044300 -1.20262900O -1.27079200 -1.12173800 -2.27694500N -2.75121100 -1.55457400 -0.60265800H -2.92623600 -1.40414000 0.38289100C -3.11178800 -2.86552300 -1.13718200H -2.30495800 -3.59271100 -0.98745300H -4.01854700 -3.21159700 -0.63486500H -3.30337900 -2.77534200 -2.20827400C -0.42996700 0.31152200 0.76247200H -0.29855400 1.35349400 1.09958100C 2.05545900 0.63324300 0.08026400C 3.15308300 -0.21541800 -0.22682800C 4.40998400 0.28528200 -0.58974800C 4.55590600 1.66732500 -0.64437100C 3.47668600 2.53030700 -0.34911000C 2.23074500 2.02960500 0.00965700C 0.93183100 -0.21181300 0.40607200C 1.37780500 -1.51479800 0.29197000H 5.23913500 -0.37882400 -0.82087400H 5.51746800 2.09106700 -0.92206600H 3.62485600 3.60527500 -0.40852200H 1.40553500 2.70586900 0.21961900N 2.71015200 -1.51215800 -0.08850200H 3.25651600 -2.35183800 -0.21534000S 0.55415400 -3.07289700 0.48017700H 0.49139700 -3.06379100 1.83196400C -1.11702200 -0.32796200 1.95224800O -0.59914900 -1.04670500 2.78240400H -2.18269600 -0.03130700 2.07523800 SCF energy=-1461.4176214C -2.41674200 2.65164600 -0.08352400O -1.34184500 3.25245100 -0.10718300C -3.73422400 3.36479400 0.15647100H -3.87606600 4.11050400 -0.63265800H -4.59963200 2.69474600 0.17198000H -3.67880300 3.90048100 1.10934200N -2.48676200 1.29962200 -0.27414800H -3.37582000 0.82657200 -0.19503500C -1.29668000 0.51014900 -0.57351100H -0.68582600 1.10435000 -1.25868900C -1.63858300 -0.75880200 -1.39073100O -1.05449600 -0.97625600 -2.44747900N -2.64672900 -1.54490200 -0.92025500H -2.84204000 -1.48248300 0.07336000C -2.99454200 -2.78257100 -1.60847300H -2.20119900 -3.53438200 -1.51260600H -3.91977200 -3.17349700 -1.17786700H -3.14690700 -2.57837100 -2.67056100C -0.35937200 0.34988900 0.65871900H -0.22472500 1.36666300 1.04195600C 2.13757900 0.61155200 0.03071000C 3.22436100 -0.26825900 -0.22047100C 4.49896600 0.19746000 -0.56864800C 4.67081600 1.57371100 -0.66353700C 3.60173700 2.46613500 -0.42224200C 2.33818500 2.00175300 -0.07961300C 0.99595000 -0.20725300 0.35170800C 1.41506900 -1.52179600 0.28948600H 5.32049400 -0.48839500 -0.75887600H 5.64600200 1.97101100 -0.93206500H 3.77238800 3.53540600 -0.51213300H 1.52041100 2.69907900 0.08532300N 2.75569900 -1.55329100 -0.04860900H 3.28251100 -2.40644200 -0.17015800S 0.52731000 -3.03046000 0.54856600H 0.70363500 -3.11282000 1.89056700N -1.00285600 -0.34615400 1.87223500O -0.31747700 -0.43664300 2.88010800O -2.17645700 -0.72235600 1.80060900 SCF energy=-1487.9649965C -1.78872900 2.74637700 -1.37439800O -0.65257700 3.21577600 -1.41601900C -3.02412100 3.62469300 -1.49088800H -3.04325500 4.06820000 -2.49241600H -3.96394500 3.08766700 -1.32539400H -2.94673000 4.44454500 -0.77043700N -2.01966400 1.40788100 -1.22071100H -2.97428500 1.07504300 -1.21234100C -0.94491000 0.40889400 -1.23544000H -0.23141900 0.70222700 -2.00880000C -1.55637400 -0.91486700 -1.72650700O -1.19840300 -1.42589500 -2.78292800N -2.58822200 -1.41299900 -0.97832400H -2.63280200 -1.13213800 -0.00474200C -3.21248800 -2.68211300 -1.33459800H -2.52213500 -3.52384200 -1.19906500H -4.09481700 -2.82693800 -0.70607700H -3.51605200 -2.65586500 -2.38367700C -0.12503200 0.41887100 0.11639700H 0.13347000 1.47889100 0.17370600C 2.45830600 0.46934800 0.12805800C 3.53706600 -0.43702300 -0.04072900C 4.87806900 -0.03759900 0.02411100C 5.13237700 1.30858100 0.26216300C 4.07703400 2.23188700 0.43137400C 2.74912700 1.82718800 0.36659800C 1.22078300 -0.27627300 0.00156000C 1.59835600 -1.58694600 -0.24577500H 5.68823600 -0.75011000 -0.11007000H 6.16070300 1.65661500 0.31432300H 4.30947600 3.27846300 0.60878800H 1.95269200 2.55719800 0.48069900N 2.98501400 -1.67820700 -0.26024600H 3.48336900 -2.50799700 -0.54796200S 0.67736000 -3.06842100 -0.57975400H 0.99573300 -3.71395400 0.57129100C -0.93920700 0.15228100 1.38486200C -1.58413900 1.23768400 2.00532700C -1.07442600 -1.11192000 1.98079500C -2.34880200 1.06698100 3.16200000H -1.46979700 2.23368500 1.58520500C -1.83763400 -1.28823000 3.13959000H -0.57771300 -1.96673300 1.53706400C -2.48210400 -0.20072700 3.73415900H -2.82936200 1.92730400 3.62149700H -1.91962700 -2.27867200 3.58117000H -3.07048100 -0.33716200 4.63790300 SCF energy= -1216.7725C 3.11456900 -1.39632900 0.01706100O 3.87603400 -1.91424800 0.82707100C 3.45499400 -1.28093600 -1.45890900H 2.81084800 -1.93497900 -2.06014300H 3.33461300 -0.25789900 -1.83274600H 4.49095700 -1.59528400 -1.59286300N 1.90089500 -0.88875600 0.42883500H 1.68485900 -1.03794600 1.41034200C 0.99568100 1.27085500 -0.48137800O 0.31006100 1.90176300 -1.29819400N 1.90225000 1.85589700 0.32291300H 2.39411700 1.26467200 0.98026800C 2.11397800 3.29670300 0.35148100H 2.07940400 3.68910000 -0.66745400H 1.34249800 3.80104900 0.94552700H 3.09406700 3.50145700 0.78830500C 0.85966100 -0.26603200 -0.37403600H 0.92010000 -0.63889900 -1.40110100C -0.51434500 -0.71912500 0.19730800C -1.74130500 -0.29883500 -0.68972100H -0.47800200 -1.81753800 0.21047600H -1.37362900 0.13133300 -1.62208300C -2.66497000 0.72911100 -0.00377200O -3.58802200 0.37601100 0.72469300N -2.40172300 2.02383200 -0.30412300H -1.54622200 2.28463400 -0.78758000H -2.93682800 2.73408200 0.17881700S -2.83040000 -1.73501100 -1.12710600H -1.97621000 -2.24740100 -2.04363600O -0.55617100 -0.24537400 1.53297500C -1.31900800 -1.04845000 2.44659500H -0.94282400 -2.08154300 2.45034800H -1.17004900 -0.60180200 3.43218300H -2.38200100 -1.03666700 2.19153100 SCF energy=-1236.2112237C -3.06381500 -1.52626100 0.05982300O -3.74876100 -2.18083200 -0.71881100C -3.40985700 -1.40891600 1.53523200H -2.70905100 -1.99569300 2.14281500H -3.37752100 -0.37390300 1.89333300H -4.41289900 -1.81264700 1.68124800N -1.94882600 -0.84863900 -0.39057600H -1.65601300 -1.07937300 -1.33985300C -1.10174500 1.33642800 0.49118200O -0.35308800 2.03167500 1.19269800N -2.14873200 1.85427100 -0.18257600H -2.69901800 1.21502700 -0.74304100C -2.46378500 3.27584300 -0.16762200H -2.39555400 3.65883800 0.85384300H -1.76860300 3.84570500 -0.79586500H -3.48030700 3.41458900 -0.54221300C -0.91570900 -0.19566000 0.40006700H -0.98164000 -0.53799900 1.43805000C 0.47919200 -0.70814000 -0.11869200C 1.66633700 -0.25063500 0.83257900H 0.40324400 -1.78583500 0.05143800H 1.22460300 0.22206000 1.71088800C 2.67873900 0.73810200 0.22229500O 3.60689300 0.36944300 -0.49497700N 2.47363500 2.03455900 0.56298900H 1.59208400 2.32041200 0.98158300H 3.06759800 2.73357800 0.13505700S 2.60080300 -1.68735800 1.52833100H 3.48157800 -1.76692300 0.50681200N 0.57725800 -0.58575800 -1.56946700C 0.74484300 0.73074600 -2.18864900H 0.14180600 1.48393900 -1.67732200H 1.78854200 1.07441100 -2.20913400H 0.39153600 0.67107600 -3.22582800C 1.41785900 -1.59704500 -2.21616500H 1.19113700 -1.60905600 -3.28903000H 2.49394900 -1.40390300 -2.09114500H 1.18565000 -2.58666800 -1.80909500 SCF energy=-1561.8410692C -2.71617600 -1.73669000 -0.41789300O -3.43761100 -2.18716100 -1.30011000C -2.80443900 -2.21023400 1.02265100H -1.89199200 -2.74016900 1.32201300H -2.95237700 -1.37889500 1.72157100H -3.64863200 -2.89702900 1.09749200N -1.79574600 -0.74888200 -0.71551500H -1.72630400 -0.54217300 -1.70870000C -1.11291700 1.29356600 0.59221500O -0.32192800 1.92457600 1.29559300N -2.30916300 1.78431500 0.20191500H -2.88158900 1.21386500 -0.40600600C -2.73353500 3.13539500 0.54309200H -2.14525300 3.88386700 -0.00009700H -3.78841900 3.24698100 0.28316200H -2.60215900 3.30820400 1.61475100C -0.79370700 -0.15982100 0.15835500H -0.75874100 -0.73998000 1.08456900C 0.60947700 -0.29868300 -0.47141600C 1.80464000 0.03358300 0.43396800H 0.72171800 -1.31512100 -0.85402900H 1.70944000 1.05594500 0.80081700C 3.12678400 -0.20803700 -0.31115900O 3.37963600 -1.29277600 -0.82416500N 3.98790700 0.84153600 -0.32538900H 3.73110800 1.75519000 0.01940300H 4.86240200 0.74196300 -0.82492700S 1.81248800 -1.01745500 1.95857100H 2.30131100 -2.11592200 1.34059500Cl 0.68512700 0.76542300 -1.97789700 SCF energy=-1215.5555852C 3.28068100 1.04578500 -0.07921000O 4.33387100 0.96854000 -0.70163100C 3.04805700 2.10608300 0.98359400H 2.10161800 2.64078700 0.84749600H 3.04041300 1.65602100 1.98427800H 3.87190500 2.81920300 0.93074800N 2.26000500 0.15071000 -0.33316700H 2.55348800 -0.59637500 -0.95276800C 0.71333600 -1.49479500 0.73905400O 0.32846400 -1.78509900 1.86957100N 0.95256000 -2.42415700 -0.22851200H 0.88318300 -2.10619000 -1.18793300C 0.55684300 -3.81398300 -0.00844800H -0.53450200 -3.91801400 0.00185700H 0.98008400 -4.42743600 -0.80754800H 0.95281400 -4.14939600 0.95159300C 1.01286900 -0.01434200 0.41219600H 1.15180700 0.42110900 1.40381000C -0.16491100 0.78269000 -0.24280900C -1.51519900 0.62277900 0.51276400H 0.13036000 1.83421200 -0.13915200H -1.29614700 0.27289000 1.52724700C -2.36760300 -0.49658600 -0.12072000O -1.81209600 -1.38912400 -0.76018700N -3.69501300 -0.49118600 0.13713300H -4.14795300 0.34408900 0.48458000H -4.26119800 -1.20445300 -0.30392200S -2.42155400 2.23663700 0.71914800H -2.38071000 2.26206600 2.06864300C -0.32963100 0.59757000 -1.74942900O -1.19337000 1.17314000 -2.37668500H 0.41525700 -0.03313600 -2.27397600 SCF energy=-1306.7672886C 3.28309500 1.19258000 0.05440500O 4.19531300 1.43452800 -0.72683200C 3.46642000 1.26111600 1.56085200H 2.83139000 2.03787300 2.00528100H 3.22090100 0.31006800 2.04731400H 4.51048200 1.50646300 1.75987400N 2.02864600 0.86901900 -0.42780000H 1.99406400 0.75279000 -1.43490000C 0.93461200 -1.14362700 0.71713200O 0.52400800 -1.47556300 1.83193200N 1.46018800 -1.99510000 -0.18593000H 1.58697500 -1.64938300 -1.12893400C 1.39953200 -3.43863900 0.00891800H 0.38282900 -3.81488100 -0.15508400H 2.08768300 -3.91710500 -0.69201000H 1.70083300 -3.67630100 1.03118400C 0.91119300 0.36561100 0.35163300H 0.95783700 0.84838600 1.33227700C -0.44289400 0.86584100 -0.21131300C -1.67875800 0.48317600 0.64818700H -0.37392400 1.95617500 -0.25378200H -1.29839100 0.21904900 1.64007600C -2.35759700 -0.81247600 0.14437900O -1.68822200 -1.64564100 -0.45566000N -3.65433100 -0.99679900 0.48410800H -4.22265400 -0.22939300 0.81663600H -4.11058500 -1.83497400 0.14794200S -2.83501500 1.91880700 0.89018100H -2.64505500 2.03970000 2.22111900N -0.69382300 0.51503900 -1.68148800O -1.77761500 0.86543200 -2.12967600O 0.20395100 -0.00825400 -2.33817300 SCF energy=-1627.9777141C 3.11996500 1.28153400 -1.21085900O 4.09603800 0.63295100 -1.57079200C 3.15405300 2.79402500 -1.08119300H 2.46500700 3.26929100 -1.79058900H 2.87689600 3.12536700 -0.07391100H 4.16911700 3.12686200 -1.30201800N 1.93101200 0.63920500 -0.92515200H 1.99193000 -0.37054000 -0.98803600C 0.74996400 1.43146600 1.19014700O 0.09735600 2.36219600 1.66985000N 1.52788400 0.60682400 1.91964700H 1.95835900 -0.17988900 1.45310700C 1.53497800 0.64755100 3.37644100H 0.61298200 0.21963600 3.78698200H 2.39551100 0.08116000 3.73983100H 1.61594400 1.68462100 3.71025000C 0.73519000 1.23291800 -0.34770300H 0.67274900 2.25844900 -0.72231400C -0.56139800 0.55775700 -0.89841000C -1.85860100 1.26531200 -0.39849200H -0.51275100 0.71478900 -1.98235500H -1.58384100 2.27003600 -0.06643300C -2.41343100 0.57217300 0.86319800O -1.71061600 -0.22673300 1.47708000N -3.64336300 0.95167700 1.27827100H -4.26585000 1.46282200 0.66716900H -4.02651600 0.49786900 2.09718300S -3.14068500 1.48374200 -1.72774000H -2.91960600 2.80099800 -1.92575000C -0.73475300 -0.95482200 -0.77021000O -1.67640400 -1.56119200 -1.19495300O 0.38681800 -1.58641400 -0.21614700C 0.39581200 -2.95864700 -0.06667700F -0.60048600 -3.39919900 0.70246200F 0.35067900 -3.59341500 -1.24602300F 1.56270700 -3.25931300 0.52951800  SCF energy=-573.94453C -2.31808100 -0.55352200 -0.19672700O -2.68370800 0.45901200 -0.79521800C -3.30862400 -1.60957400 0.26783400H -3.82181500 -2.02016900 -0.60820300H -2.84564200 -2.42870700 0.82714100H -4.06611900 -1.13070000 0.89653400N -1.01085200 -0.79358700 0.10289000H -0.71422100 -1.70317300 0.44521600C 1.38048500 -0.75001000 -0.13481100O 1.36057500 -1.93798600 0.19001300N 2.52810600 -0.06215500 -0.33834000H 2.45464300 0.93969900 -0.46313200C 3.83884700 -0.66813900 -0.14851500H 3.88025300 -1.62791100 -0.66985000H 4.59735500 0.00020100 -0.56282700H 4.05192600 -0.84434200 0.91284100C 0.07274000 0.05142100 -0.39574600C 0.09666900 1.44202000 0.19710200C -0.19590900 2.62824500 -0.66866900H 0.13659800 2.47974900 -1.70389200H -1.28170200 2.81827900 -0.71634700H 0.27996100 3.53858100 -0.27961500C 0.00402500 1.58669400 1.68563700H 0.45606800 0.74054300 2.21758800H 0.49112400 2.50941300 2.02777100H -1.04760600 1.64483300 2.01753900H -0.02745300 0.14286500 -1.48760500 SCF energy=-613.2517585C -2.14416400 -1.55501000 -0.19277900O -2.82770200 -2.27113900 -0.91717900C -2.52697900 -1.24892000 1.24377300H -1.85584600 -1.77168000 1.93704600H -2.46988100 -0.18007400 1.47537500H -3.54466200 -1.60560500 1.40906500N -0.97960600 -0.98681000 -0.67235800H -0.69325700 -1.36610700 -1.56931300C -0.32605600 1.21440700 0.38592300O 0.19132600 1.80872700 1.32926900N -1.17680300 1.79427400 -0.49592200H -1.62273600 1.19615200 -1.17949500C -1.58238400 3.18774000 -0.37606400H -0.70151500 3.81901900 -0.23133200H -2.09450700 3.48496800 -1.29429500H -2.25506600 3.33931000 0.47682100C 0.03878600 -0.27482700 0.10427900H 0.15229800 -0.72619100 1.09700500C 1.35664300 -0.30365300 -0.61219300H 1.33729400 -0.17273100 -1.69448100C 2.66242800 -0.25059800 0.12345600H 2.54732200 0.46260900 0.95565500C 3.01960500 -1.62292600 0.74799400H 3.93410700 -1.54081000 1.34842100H 2.22195500 -1.98972500 1.40455500H 3.18847900 -2.37513700 -0.03235400C 3.79753400 0.24687700 -0.78575400H 3.94425400 -0.43170200 -1.63672400H 3.58121100 1.24615900 -1.18135600H 4.74394300 0.30005500 -0.23516000 SCF energy=-570.5334254C -2.48238500 -0.47137000 -0.05400000O -3.31701100 -1.31404400 0.26090400C -2.85034300 0.75068000 -0.88253300H -2.43855300 1.67869100 -0.47123900H -2.47012000 0.64389700 -1.90689400H -3.93846800 0.81988300 -0.92335600N -1.16881500 -0.60370100 0.32397200H -0.91074100 -1.49757900 0.73761300C 1.23663000 -0.64293200 -0.00123600O 1.20871200 -1.79811200 0.41235800N 2.36019200 -0.02593600 -0.44165800H 2.31412300 0.97004100 -0.62044100C 3.66715900 -0.66629700 -0.35898200H 3.58845800 -1.69764000 -0.70982600H 4.36658500 -0.12055100 -0.99693500H 4.04911100 -0.68033300 0.66960900C -0.05461900 0.23104400 -0.06926000H -0.15797200 0.55460800 -1.11997000C 0.07884600 1.44867200 0.79891200H -0.64451100 1.67982000 1.57506500O 0.79011100 2.47943600 0.22068600H 0.87622800 3.21960100 0.84117600 SCF energy=-573.9253383C -2.25348200 -0.44190500 0.02901100O -3.22150300 -0.61482600 0.76403200C -2.25154300 -0.86786700 -1.42803600H -2.28214300 0.00953700 -2.08627800H -1.35974700 -1.44705300 -1.69177500H -3.14388800 -1.46933100 -1.60745800N -1.10920300 0.15420000 0.51402400H -1.20906900 0.49119400 1.46660700C 1.12769700 -0.63447800 -0.31065300O 1.98707600 -0.63559600 -1.18980000N 1.04057800 -1.59696700 0.64493300H 0.21788800 -1.60027300 1.23365200C 1.92427800 -2.75462700 0.65193300H 2.95488700 -2.42848800 0.49293300H 1.84645800 -3.25213600 1.62174200H 1.66529000 -3.46708900 -0.14134200C 0.10184500 0.51596600 -0.21795000H -0.15433100 0.76131800 -1.25319400C 0.73621700 1.80424800 0.42933900H 0.87748800 1.56869900 1.49708100C -0.23856700 2.99276600 0.30653300H -0.36929500 3.27222300 -0.74667600H -1.22746300 2.76837700 0.71983700H 0.16253700 3.86356500 0.83559800C 2.06664700 2.15451400 -0.15533500H 2.97958600 1.68848400 0.19789100H 2.11904300 2.73202100 -1.07422000 SCF energy=-609.8395341C 2.44444800 -0.15282400 -0.33124200O 3.18381900 -0.39440700 -1.27956100C 2.88088800 -0.33853800 1.10976900H 2.80488900 0.59627600 1.67844100H 2.26249300 -1.09033200 1.61252300H 3.92109500 -0.66726200 1.10427400N 1.17045900 0.33285100 -0.56373300H 0.92231600 0.30287900 -1.54797400C -0.78629000 -0.83472400 0.40705800O -0.54757900 -1.71355600 1.23264300N -1.71837400 -0.97566300 -0.56998500H -1.95221400 -0.16991500 -1.13542400C -2.56733400 -2.15773500 -0.64659100H -3.29164600 -2.18571500 0.17649700H -3.10160700 -2.14530700 -1.59982400H -1.94967000 -3.05750300 -0.59014900C 0.07854300 0.44983300 0.39247600H 0.50287800 0.49764400 1.39509400C -0.67365000 1.80028600 0.18359600H 0.08881100 2.56722200 0.41052100C -1.20258600 2.06731200 -1.18792000H -0.53008100 2.32163100 -2.00184500H -2.27271200 2.15599000 -1.35408600O -1.70120800 1.81666200 1.17381500H -2.09351500 2.70282700 1.20993700 SCF energy=-723.2452066C 3.14488500 0.56829100 -0.29108900O 4.02787600 0.44646500 -1.13292100C 3.44464600 0.77707500 1.18096500H 2.98957000 1.70120900 1.55874200H 3.06215900 -0.06014700 1.77437600H 4.52744900 0.84350800 1.29620300N 1.81896600 0.54604400 -0.68412700H 1.70866300 0.29681900 -1.66304900C 0.28839400 -1.04827400 0.39229400O 0.95750100 -1.68745600 1.20398400N -0.68481600 -1.61118500 -0.36540200H -1.33463100 -1.03148200 -0.88690400C -1.02398700 -3.02174200 -0.20900400H -1.44395600 -3.22468500 0.78331400H -1.75604000 -3.28763600 -0.97454700H -0.12805100 -3.63635300 -0.33074700C 0.63409200 0.44506900 0.15692900H 0.89179900 0.83212800 1.14478100C -0.48618300 1.34561700 -0.44876700C -1.71889500 1.45545500 0.37467600H -0.73805200 1.00349500 -1.45896300H -0.03440500 2.34209600 -0.54930000H -1.70502500 1.99783200 1.31598300C -2.97013300 0.86430800 -0.05067900O -3.09824100 0.12516000 -1.02747600O -4.01816400 1.19332600 0.74591500H -4.80721100 0.74444300 0.38885800 SCF energy=-613.2470607C -2.20512800 1.41737600 0.04420600O -2.97557300 1.98568500 0.81329300C -2.54414700 1.18780800 -1.41869300H -1.92087900 1.81955100 -2.06407100H -2.38825400 0.14717700 -1.72404900H -3.58984000 1.45914900 -1.57071400N -0.98603900 0.95799500 0.49003700H -0.77791600 1.20863100 1.45247600C 0.08012100 0.32366100 -0.28199600H 0.03815500 0.68667900 -1.31314800C 1.46124600 0.76256800 0.30658300C -0.06034800 -1.21338000 -0.38450700O 0.59989600 -1.85091800 -1.20490500N -0.92943400 -1.80027900 0.47575100H -1.48706200 -1.20116400 1.06935400C -1.16734100 -3.23683100 0.46594700H -0.22151200 -3.77806800 0.56244800H -1.81667800 -3.48966600 1.30718700H -1.64539800 -3.55379000 -0.46817300H 1.40593400 1.86001300 0.36119800C 2.63854700 0.42574400 -0.65630900H 2.36608400 0.77549500 -1.66167900H 2.75000300 -0.65999500 -0.73086400C 1.68050200 0.22930400 1.68854900H 2.15936500 0.83377300 2.45240700H 1.55123900 -0.82982900 1.89714500C 3.96145400 1.07356700 -0.23248800H 3.87050100 2.16551300 -0.15848900H 4.30408000 0.69965200 0.73951900H 4.74648200 0.85581800 -0.96591900 SCF energy=-857.9739391C -1.94983800 2.52949300 -0.12515500O -0.76023400 2.77521800 -0.34994800C -2.98870100 3.63452500 -0.03751000H -3.01085100 4.17230200 -0.99123700H -3.99503600 3.26996700 0.19084000H -2.68320500 4.34839100 0.73435000N -2.40656600 1.26529900 0.07658800H -3.40252600 1.06272000 0.12015100C -1.57503400 0.08959900 -0.10715300H -1.06157700 0.16930000 -1.07447500C -2.54440300 -1.11974100 -0.16364700O -3.76791000 -0.93157800 -0.19034700N -1.98693200 -2.34318100 -0.19756100H -0.96847200 -2.45636600 -0.08339200C -2.81506900 -3.53934000 -0.25177700H -3.45771600 -3.52663900 -1.13824300H -2.15503100 -4.40894000 -0.29532200H -3.45905600 -3.61765800 0.63182900C -0.47963600 -0.02160800 1.01418000H -0.88606900 -0.60772200 1.84845600H -0.29020500 0.99131800 1.37330400C 2.01824300 0.05885600 0.24744200C 2.98427100 -0.94639400 -0.03373200C 4.29761900 -0.64875100 -0.34702800C 4.65914700 0.71268700 -0.36707600C 3.72494000 1.72636900 -0.09593300C 2.39841100 1.41579600 0.20907200C 0.80125100 -0.62822100 0.54287000C 0.98389200 -2.05940600 0.30463800H 5.03008600 -1.42270600 -0.56123700H 5.68636600 0.98132300 -0.59922000H 4.03795100 2.76559300 -0.13979200H 1.66091300 2.19634300 0.37303500N 2.30287200 -2.18368800 0.04151200H 2.72339800 -3.05855800 -0.24560400 SCF energy=-781.7859506C 2.70481100 -1.92606600 -0.15172700O 3.76440500 -2.43282400 0.20800200C 1.69511100 -2.68633600 -0.99683200H 0.69569000 -2.67627900 -0.54849800H 1.61379900 -2.24288300 -1.99789200H 2.04082700 -3.71616500 -1.09825200N 2.39141300 -0.63541000 0.18998600H 3.11581500 -0.10551400 0.67021200C 1.56178300 1.63166000 0.04952100O 2.60051700 1.97072700 0.60881300N 0.63969900 2.51660100 -0.40580000H -0.25467700 2.16355500 -0.72213300C 0.77870900 3.94981800 -0.17671600H 1.79357700 4.26361000 -0.43149200H 0.06639900 4.47692900 -0.81576400H 0.58967900 4.21307300 0.87147100C 1.21788800 0.12804800 -0.19664900H 1.04133300 0.01838300 -1.27442100C -0.01206100 -0.25776100 0.58729100H 0.20071200 -0.52728700 1.61734300C -1.33920900 -0.28805500 0.10676900C -2.44289600 -0.53726200 1.00878500C -1.67010000 -0.09240600 -1.27286400C -3.74769700 -0.61732500 0.50684500C -2.97060200 -0.16928500 -1.74390400H -0.86977700 0.08284500 -1.98636500C -4.01934200 -0.44053600 -0.84974000H -4.56432600 -0.81340100 1.19919100H -3.17335400 -0.03159900 -2.80231000H -5.04337600 -0.50530700 -1.20667400N -2.20900800 -0.74985500 2.36300500H -1.43341400 -0.25294700 2.78251800H -3.03138300 -0.73654500 2.95353000 SCF energy=-860.3976911C 3.44402100 -1.56484000 -0.55809900O 4.18790400 -2.38051200 -0.02029500C 3.75427300 -0.94826200 -1.90929500H 2.96335100 -1.16500900 -2.63816100H 3.85373500 0.13938100 -1.82876300H 4.69191000 -1.37730800 -2.26594800N 2.26309900 -1.20656600 0.05696000H 2.16946900 -1.59930500 0.98870200C 1.83554200 1.19474000 0.38713600O 2.69962500 1.89019500 -0.14177800N 1.31181900 1.46155000 1.61075400H 0.49259800 0.93852100 1.89260700C 1.68985700 2.64516200 2.37104100H 1.24181100 3.55522400 1.95276100H 1.35784600 2.52197300 3.40500500H 2.77636900 2.75672600 2.35102900C 1.34968600 -0.12228700 -0.29892200H 1.47346200 0.07545900 -1.36907500C -0.07069800 -0.53313300 -0.01185000H -0.21573000 -1.53181000 0.38736000C -1.21354700 0.19476400 -0.41382800C -2.54524500 -0.31800100 -0.16749500C -1.10279800 1.41538800 -1.14776200C -3.64215500 0.33744800 -0.73467000C -2.21262600 2.05521600 -1.67791400H -0.11839400 1.83684700 -1.33000400C -3.48855400 1.50759100 -1.48784600H -4.64134900 -0.05380100 -0.57264300H -2.08804600 2.97117800 -2.24913300H -4.36449700 1.99731400 -1.90485300N -2.69741300 -1.49885400 0.60365300C -3.88451900 -2.30714900 0.35226800H -3.73967800 -3.29059400 0.81275600H -4.80983400 -1.87349000 0.77384500H -4.01958200 -2.44735200 -0.72353700C -2.43940700 -1.36163300 2.04039300H -3.28485400 -0.87955000 2.56353400H -2.28034100 -2.35285300 2.47997300H -1.54400100 -0.76195100 2.21261400 SCF energy=-954.3363592C 3.46345500 1.37123800 1.01986100O 4.12523200 2.37665700 0.78053700C 3.88468300 0.34508600 2.05500700H 3.12519600 0.23362400 2.83899300H 4.04322500 -0.63510800 1.59272500H 4.81437800 0.69031400 2.50971500N 2.27171600 1.16327600 0.35559200H 2.10385900 1.84907700 -0.37424700C 1.96801700 -1.00170100 -0.78831200O 2.88091200 -1.79099500 -0.55962200N 1.40775500 -0.84339800 -2.01371800H 0.56496200 -0.28664600 -2.08286200C 1.81881400 -1.64579800 -3.15886600H 1.46463200 -2.68038700 -3.07354800H 1.40939200 -1.19753400 -4.06730600H 2.90951100 -1.66013200 -3.22226900C 1.44938400 -0.04419800 0.33572800H 1.64319400 -0.58957900 1.26364700C -0.00453000 0.33080200 0.23581700H -0.22088300 1.36678400 0.01342300C -1.07969500 -0.56575000 0.45125800C -2.47247700 -0.18579200 0.37481300C -0.80562500 -1.92322300 0.81433400C -3.46400900 -1.12018500 0.69448100C -1.81103600 -2.83105700 1.10245300H 0.22559800 -2.25557100 0.87664200C -3.15458400 -2.43310700 1.05125300H -4.49825200 -0.79530200 0.65066900H -1.55149600 -3.85090300 1.37425200H -3.94955300 -3.13583900 1.28304400C -3.00794500 1.15507100 -0.01943500O -4.13325300 1.53380500 0.25224600O -2.15498700 1.91298100 -0.75109100C -2.66200700 3.20007900 -1.16070000H -3.54620000 3.07518900 -1.79061000H -2.92232000 3.80163600 -0.28640800H -1.84943300 3.66286500 -1.72169300  SCF energy=-930.9497458C 3.44063100 -1.42388400 -0.66120400O 4.23537700 -2.22666000 -0.18486500C 3.69354100 -0.70508400 -1.97329700H 2.91234500 -0.93336000 -2.70929500H 3.72052100 0.38071300 -1.83140000H 4.65420200 -1.04650600 -2.36157600N 2.24757500 -1.17381300 -0.00975300H 2.18790800 -1.63490300 0.89324400C 1.70138600 1.20079100 0.44968800O 2.39857500 2.03727500 -0.11836500N 1.30671500 1.31155000 1.74143600H 0.64218900 0.64035600 2.10577100C 1.67840700 2.45561700 2.56591700H 1.19039800 3.37250900 2.21584700H 1.37659000 2.25549000 3.59628400H 2.76065300 2.60591500 2.52840600C 1.28228700 -0.11551900 -0.28961900H 1.36547900 0.13558000 -1.34991600C -0.10730800 -0.58420700 0.03880700H -0.19230800 -1.47984000 0.64009600C -1.28524600 0.06978600 -0.39179500C -2.62052600 -0.36779800 -0.08364700C -1.20660100 1.21915000 -1.24231000C -3.74735100 0.24969900 -0.62047500C -2.33134200 1.84703400 -1.75022100H -0.22968200 1.61165000 -1.50364300C -3.61379300 1.36266300 -1.44958900H -4.72489100 -0.14206000 -0.36519300H -2.21397500 2.71848700 -2.38836800H -4.49823200 1.84944700 -1.84866300N -2.88646600 -1.48205100 0.83379000O -3.95280900 -2.08783600 0.70669600O -2.04745000 -1.74437400 1.70485500 SCF energy=-1252.1635704C 3.56752700 1.58839700 1.37415400O 3.89604300 2.76640000 1.46084900C 4.39221700 0.46467300 1.97348000H 3.81255300 -0.10858800 2.70779500H 4.73840500 -0.22664000 1.19757200H 5.25242900 0.91167900 2.47390600N 2.38684100 1.25306700 0.73818200H 1.94204300 2.05068600 0.29333600C 2.52072100 -0.42270800 -1.07689800O 3.60624300 -0.98844500 -1.17586100N 1.80017400 0.00239900 -2.14387100H 0.85995300 0.34230400 -1.98586500C 2.25456700 -0.20396700 -3.51400400H 2.19201500 -1.26019300 -3.80156500H 1.62932900 0.39108700 -4.18346800H 3.29472600 0.11748000 -3.60919900C 1.93634600 -0.07559900 0.33371100H 2.40714300 -0.80045200 1.00279900C 0.43781400 -0.16400700 0.43129400H -0.08484600 0.77212800 0.57525500C -0.29640300 -1.37325300 0.38700600C -1.73644000 -1.44678000 0.49267900C 0.39721700 -2.62224100 0.30362900C -2.37098800 -2.69237800 0.58712500C -0.25999700 -3.83977600 0.36539600H 1.47754500 -2.62079400 0.20340900C -1.65327400 -3.88582500 0.52221600H -3.45084900 -2.70990200 0.69255600H 0.31291500 -4.76088000 0.30013000H -2.17307900 -4.83714900 0.58279200C -2.67896400 -0.30142800 0.50169100O -3.78839600 -0.30050200 0.96832100O -2.16601100 0.81830100 -0.18178700C -2.93105500 1.95484200 -0.29398800F -3.23134200 2.49056900 0.89671100F -4.06650800 1.74574800 -0.97315400F -2.18861100 2.84204400 -0.97986300 SCF energy=-649.1965311C 2.35420700 -0.56252500 0.21976300O 2.59870900 0.15636000 1.19924500C 3.43940300 -1.38555500 -0.44658600H 3.85935100 -2.07892000 0.28947100H 3.08527100 -1.95337600 -1.31240200H 4.24455700 -0.71414400 -0.76200600N 1.10537300 -0.66746100 -0.29961200H 0.90445600 -1.26146700 -1.09699200C -1.29747300 -0.63826200 -0.31458900O -1.29882000 -1.10681500 -1.45530000N -2.35716000 -0.63714600 0.52062900H -2.16796400 -0.37983400 1.48211500C -3.61875900 -1.27690000 0.17789800H -3.82347100 -1.11748200 -0.88276100H -3.59020000 -2.35783900 0.36620400H -4.41910100 -0.82998500 0.77351300C -0.03262600 0.08757700 0.23287100C -0.04352400 1.53035900 -0.25395600C -0.87259600 2.53973100 0.47896500H -1.04553900 2.25539700 1.51992600H -0.37949300 3.52155600 0.46738900H -1.85843400 2.68432400 -0.00007400C 0.37925600 1.84774300 -1.65417100H -0.42687900 1.63812600 -2.38033600H 0.62681600 2.91212800 -1.74942600H 1.24870100 1.26370800 -1.97235700O -0.07087600 0.00294100 1.64661300H 0.82500300 0.27715100 1.94497800  SCF energy= -688.4934009C 2.32133100 -0.51801300 -0.15965100O 2.75530100 0.40778600 0.51798500C 3.25106300 -1.48668600 -0.87761100H 3.94305500 -0.91070000 -1.49997800H 3.84918800 -2.02030700 -0.13119100H 2.72974500 -2.21864200 -1.50263800N 0.98307400 -0.77650800 -0.30923800H 0.67886500 -1.47163400 -0.98494200C -1.39201000 -0.49649900 -0.49764800O -1.33997300 -1.22187900 -1.49300400N -2.54235000 -0.10337300 0.08980700H -2.46268200 0.48994100 0.90590500C -3.85619000 -0.44227000 -0.43485300H -3.81062600 -1.42746200 -0.90423700H -4.57760800 -0.46422300 0.38628800H -4.19031200 0.28463800 -1.18608800C -0.09345600 0.06921800 0.19416200C 0.06475800 1.53079000 -0.17737500C 0.24952100 2.58869700 0.86300000H -0.28814100 2.36938300 1.78950000H 1.31550500 2.68036300 1.13137900H -0.08043500 3.56394600 0.48127300C 0.35042600 1.86162000 -1.61010400H 0.00057400 1.08938100 -2.30391700H -0.12075200 2.81293700 -1.89197600H 1.43425300 1.98813500 -1.78054200O -0.25192000 -0.00201900 1.60730600C -0.24226500 -1.30447100 2.18429000H -0.44809400 -1.15706600 3.24694200H -1.01905800 -1.95064300 1.75032900H 0.73512000 -1.78430500 2.06634900 SCF energy= -707.9263308C -2.40147000 -0.44316200 0.36494000O -2.84310200 0.63655600 -0.01788300C -3.32757900 -1.53120700 0.89536600H -3.99128300 -1.85131300 0.08471500H -2.80323700 -2.40708700 1.29070500H -3.95618200 -1.10318500 1.68237600N -1.07539900 -0.77311200 0.35970600H -0.78533000 -1.68956600 0.68908400C 1.29486500 -0.67826200 0.50158900O 1.26522500 -1.88379400 0.76783100N 2.41866200 0.06178400 0.62795700H 2.34195300 1.06086100 0.48869800C 3.66017400 -0.50060400 1.14257900H 3.92349400 -1.40227600 0.58292900H 4.45439900 0.24062900 1.02762400H 3.56732100 -0.77051700 2.20135500C 0.03757700 0.04615300 -0.12848100C -0.08764900 1.48539500 0.35092700C -0.59343900 2.59533600 -0.52042300H -0.82047600 2.25382400 -1.53159100H -1.52097200 3.00817000 -0.10023400H 0.12882900 3.42752900 -0.57710800C -0.12288500 1.72320300 1.83316300H 0.36544300 0.93306900 2.41380200H 0.35208800 2.68066300 2.09228400H -1.16607500 1.79205600 2.18541600N 0.12085300 -0.03777600 -1.60948000C 1.26914000 0.62510100 -2.22358300H 2.20897400 0.05126500 -2.12969100H 1.06170700 0.75919100 -3.29160200H 1.42796000 1.61513100 -1.79084100C -0.06761100 -1.36480600 -2.19373200H -0.98874100 -1.81805000 -1.82568600H -0.16231500 -1.24415100 -3.27845000H 0.76991000 -2.05750100 -1.99472700 SCF energy=-762.5653483C 2.34894800 0.56447700 0.00843800O 2.72744600 -0.60553700 0.00672100C 3.32836400 1.72649300 -0.00155800H 3.81806600 1.76186700 -0.98132400H 2.85916200 2.69653700 0.19102100H 4.10288300 1.54225000 0.74852900N 1.02987800 0.91118300 -0.00106300H 0.73760100 1.88447700 0.00723600C -1.37532900 0.85067800 0.04932500O -1.29443900 2.07243700 0.16492900N -2.53823600 0.17431600 0.01315900H -2.49957900 -0.81597300 -0.20166500C -3.82491800 0.85754000 0.03096600H -4.01065800 1.38926800 -0.91015100H -4.61032800 0.11474000 0.18632500H -3.84731700 1.58444300 0.84683100C -0.06611400 -0.04728600 -0.02526000C -0.04906000 -0.99227800 1.17509600C 0.34870400 -2.43459100 1.10540100H 0.05985500 -2.92151200 0.17162700H 1.44153300 -2.53673400 1.20612300H -0.11112400 -2.98980500 1.93409200C -0.02335200 -0.33642200 2.52486400H -0.47808300 0.66022100 2.52984700H -0.54702300 -0.95602900 3.26495600H 1.01160300 -0.22030300 2.89117700C -0.16263500 -0.79506100 -1.36974400O -0.95511100 -1.69605400 -1.57627000O 0.64656300 -0.30995100 -2.32369800H 0.48860100 -0.84039400 -3.12790100 SCF energy=-801.8719095C 2.24842400 -0.69697400 0.51286800O 2.67276500 -0.34957800 -0.58835600C 3.17808900 -1.19273700 1.60926100H 3.80032100 -0.35587400 1.94567200H 2.65280400 -1.61029700 2.47413300H 3.84536200 -1.95145700 1.18967200N 0.92730200 -0.65285700 0.84385500H 0.60205300 -0.95375400 1.75843000C -1.46457400 -0.42069100 0.78129700O -1.43450300 -0.93702200 1.89802800N -2.59674100 -0.04229900 0.15909000H -2.50081800 0.48851500 -0.70006800C -3.89870500 -0.14004400 0.80444700H -4.01269900 0.60776100 1.59903400H -4.67337300 0.01530600 0.05022500H -4.01804000 -1.13209100 1.24703800C -0.12988700 -0.19626400 -0.04839000C -0.20507200 -1.01903000 -1.33360200C 0.25301800 -0.52996900 -2.67304200H 0.10373700 0.54176000 -2.81902800H 1.32722400 -0.73534100 -2.81062800H -0.28673000 -1.05930200 -3.47027000C -0.34632900 -2.50316100 -1.15908000H -0.83575600 -2.78408000 -0.22013900H -0.92162100 -2.93645300 -1.98824600H 0.63896800 -3.00140900 -1.16994600C -0.06563500 1.32381000 -0.32175100O -0.82373800 1.88218100 -1.09697000O 0.83782300 1.96337400 0.42063300C 0.93614200 3.38747700 0.21309200H -0.01898500 3.86958800 0.43647500H 1.71216200 3.72185500 0.90115400H 1.21986200 3.59521300 -0.82140600 SCF energy=-666.1985694C -2.33038900 -0.58409400 0.02204600O -2.73060300 0.54978600 -0.22455600C -3.27987500 -1.74422200 0.26744300H -3.76870600 -2.00118700 -0.67905600H -2.78627900 -2.63776800 0.66213700H -4.05808800 -1.42072500 0.96442800N -0.99902500 -0.89348800 0.08925900H -0.67599600 -1.84536200 0.24378100C 1.40649900 -0.75830200 0.08077700O 1.36940700 -1.95627600 0.34398300N 2.54125500 -0.04061900 -0.00240200H 2.47163200 0.95122600 -0.18953800C 3.85449200 -0.65126200 0.17015500H 3.98088900 -1.48401700 -0.52821200H 4.61631900 0.10519300 -0.02772300H 3.97659400 -1.03156500 1.18970700C 0.07108600 0.05811200 -0.20802800C 0.02260900 1.31982900 0.64115300C -0.29591100 2.66586500 0.07182500H 0.02719900 2.78176800 -0.96770100H -1.38427200 2.84078500 0.08571300H 0.17199800 3.45781800 0.67137400C -0.07352900 1.12278500 2.12356900H 0.36188100 0.17409400 2.45750400H 0.42935700 1.93914800 2.65806700H -1.12599400 1.13033100 2.45469200C 0.08942700 0.36729000 -1.66094800N 0.15299500 0.57927500 -2.80093500  SCF energy=-1099.6989917C -0.03162200 -2.41163900 0.58585200O 0.38805000 -2.62816300 -0.54954500C 0.14820800 -3.40351600 1.72060100H 1.20520100 -3.41726000 2.00998600H -0.45485400 -3.16907700 2.60333600H -0.10853600 -4.40327800 1.35913600N -0.67133900 -1.25012700 0.91063500H -0.95449100 -1.04110000 1.86441100C -1.55110000 0.98962400 0.82262200O -1.78363000 0.82967800 2.01819300N -1.83937100 2.11440300 0.14413600H -1.58071200 2.16678000 -0.83374600C -2.43481100 3.27440600 0.79733400H -1.79456400 3.63247100 1.61008600H -2.55293900 4.06544800 0.05446500H -3.41391700 3.02034100 1.21544300C -0.88970000 -0.17103800 -0.04013300C -1.84031400 -0.56183200 -1.16917300C -1.39494700 -0.97420200 -2.53899200H -0.43697600 -0.54810100 -2.83767600H -1.29587100 -2.07011600 -2.59797700H -2.14849800 -0.67718300 -3.28232200C -3.21881800 -0.98585100 -0.75038300H -3.56357000 -0.50263800 0.17044800H -3.94554800 -0.76807500 -1.54380900H -3.26447800 -2.07505700 -0.57660400C 0.42437900 0.43798400 -0.56402900O 0.51050900 1.17820800 -1.50765100O 1.48843300 0.13262400 0.26442500C 2.73202200 0.66429900 0.00120600F 2.73265000 2.00525200 0.08358500F 3.19802600 0.30786400 -1.20052000F 3.55799600 0.18563000 0.94011400  SCF energy=-649.1697223C 2.16504100 -1.08179400 -0.29363400O 2.63084600 -1.92413300 -1.05904400C 2.99960700 -0.48575300 0.82107300H 2.91528100 0.60072200 0.88079200H 2.67361600 -0.88446100 1.78718100H 4.03615100 -0.77838500 0.64247300N 0.84176200 -0.71045500 -0.45525000H 0.41152400 -1.23043700 -1.21382100C -1.39821100 -0.44963000 0.41938100O -1.69700800 -0.82733200 1.55233600N -2.15240100 -0.70903100 -0.67355800H -1.95597400 -0.20001800 -1.52452600C -3.43835600 -1.39317400 -0.56759400H -4.20045700 -0.74763400 -0.11507900H -3.75969900 -1.69132800 -1.56815500H -3.32302800 -2.28256900 0.05523400C -0.02729900 0.28106500 0.21234200C -0.16870900 1.58498300 -0.63268800H -0.44537300 1.28281900 -1.65546100C 1.18215300 2.33261700 -0.75254600H 1.52921500 2.65976100 0.23168900H 1.94612700 1.69405900 -1.20962700H 1.05929400 3.21828500 -1.38475100C -1.23403300 2.47645800 -0.07582000H -1.78272700 3.15038200 -0.72709500H -1.32564500 2.61109900 0.99741000O 0.44186900 0.61090800 1.48345500H -0.09064800 0.06994100 2.10833700 SCF energy=-688.4640366C 2.08898200 -1.14487000 -0.43433400O 2.45181200 -2.20493500 -0.94002600C 3.10695500 -0.19108500 0.15950800H 3.78076700 0.13969300 -0.63781000H 2.67385000 0.67338900 0.65862100H 3.71236700 -0.76357100 0.87003700N 0.73291100 -0.86785800 -0.38789700H 0.20382300 -1.67332100 -0.70647200C -1.53003800 -0.29579200 0.31413200O -2.13482800 -0.16809400 1.36976500N -2.06566200 -0.95394800 -0.75870700H -1.63792800 -0.83225400 -1.66739700C -3.44642600 -1.42878000 -0.72655000H -4.16077600 -0.59652800 -0.72904400H -3.61832300 -2.06145200 -1.60056700H -3.60687600 -2.01579700 0.18023100C -0.07252000 0.26528300 0.11439600C -0.17079100 1.45437100 -0.90278900H -0.49837400 1.00859200 -1.85534700C 1.17882200 2.14671600 -1.20377700H 1.60513000 2.59122200 -0.30078000H 1.90047400 1.44844400 -1.63923100H 1.01333200 2.94869000 -1.93164700C -1.19649600 2.45362900 -0.46257000H -1.58671700 3.16958200 -1.18024900H -1.44076700 2.58285100 0.58573800O 0.43118700 0.80915000 1.30186600C 0.56672700 -0.03645400 2.45453100H 1.21730000 0.51347800 3.13863700H -0.40446800 -0.21680000 2.91792700H 1.03976900 -0.99063700 2.19544900 SCF energy=-707.8987169C 2.10019000 1.36647800 0.12305500O 2.43910500 2.54175900 0.26160500C 3.14569100 0.28901600 -0.08353600H 3.79836500 0.26238200 0.79563400H 2.72581900 -0.69631900 -0.27743700H 3.76711500 0.59953500 -0.93036500N 0.74753200 1.07542100 0.12388100H 0.21810800 1.94033400 0.14773100C -1.52355200 0.33207800 -0.34215900O -2.15542300 -0.17223000 -1.26338700N -2.04199000 1.34734400 0.41406800H -1.59526100 1.58485800 1.29004300C -3.41318900 1.80755800 0.21343900H -4.14401600 1.05769300 0.54063900H -3.55923000 2.73021100 0.78017900H -3.57778700 2.00585600 -0.84779300C -0.06640400 -0.16183000 0.02323900C -0.17322800 -0.84194000 1.45492100H -0.38976300 0.01861900 2.11627200C 1.14760400 -1.42717900 1.98981200H 1.53618800 -2.22410700 1.34994700H 1.91598400 -0.65727900 2.08839500H 0.97457200 -1.84728000 2.98753800C -1.30488600 -1.81201700 1.59871100H -2.18338600 -1.78347800 0.96334500H -1.29903500 -2.51867300 2.42338300N 0.49557700 -1.03853700 -0.99447200C -0.00504600 -2.40995900 -1.10349000H -0.03465400 -2.90132900 -0.12934800H -1.00732300 -2.46716400 -1.55244800H 0.69277800 -2.96910100 -1.73886900C 0.65220100 -0.45242700 -2.33219100H 1.40255000 -1.03726200 -2.87781300H -0.28519700 -0.45815800 -2.90598900H 1.01058500 0.57615500 -2.26392900 SCF energy=-762.5328722C -2.00379300 1.38435400 -0.31516100O -2.33200700 2.54325600 -0.55191300C -3.05554300 0.34925200 0.03197900H -2.69500900 -0.67028100 0.15950000H -3.53876300 0.67214700 0.95970000H -3.81600100 0.36176600 -0.75482500N -0.65908500 1.05856000 -0.36600300H -0.10646900 1.90441100 -0.46161700C 1.54630700 0.29223300 0.35322600O 2.07516000 -0.07641500 1.39237900N 2.16588100 1.12272200 -0.53362600H 1.77769700 1.23835300 -1.46047900C 3.54004000 1.56405500 -0.30956100H 4.25217600 0.73788800 -0.42121400H 3.77508800 2.34935100 -1.03157200H 3.63366100 1.96367000 0.70262200C 0.09882000 -0.15720500 -0.04343300C 0.23257100 -1.13891700 -1.29396900H 0.61221900 -0.47544400 -2.08610800C -1.10146300 -1.70933200 -1.80160200H -1.55478700 -2.38270300 -1.06825800H -1.81420100 -0.91934800 -2.05549200H -0.91292900 -2.28609200 -2.71371500C 1.23849300 -2.22390500 -1.07066100H 2.30372400 -2.01647000 -1.11307200H 0.92372200 -3.19624400 -0.70912900C -0.43905900 -0.87760000 1.21180400O -0.53904700 -2.07722900 1.33368800O -0.79047000 -0.00445600 2.17735000H -1.03502200 -0.52882800 2.96331300 SCF energy= -801.8400737C -1.71835000 -1.63641700 -0.63411900O -1.94523300 -2.58829200 -1.37644400C -2.86322700 -0.91289200 0.04741200H -2.57901500 -0.13769500 0.75756500H -3.48222900 -0.46557000 -0.73698200H -3.47656800 -1.65893100 0.56195800N -0.40514300 -1.24488700 -0.44720000H 0.19567900 -1.74769800 -1.09227400C 1.58342900 0.17302200 -0.46937500O 1.88704200 1.28996200 -0.86562200N 2.40034300 -0.90834800 -0.62745900H 2.20429700 -1.75624400 -0.11181700C 3.72511800 -0.76373800 -1.22421000H 4.40682900 -0.21274400 -0.56535500H 4.13016000 -1.75948700 -1.41865700H 3.64191500 -0.21712100 -2.16618800C 0.22069400 -0.11115400 0.24742000C 0.54605400 -0.44736700 1.77255200H 1.09887900 -1.39704900 1.70364700C -0.69340500 -0.72361300 2.63884000H -1.30750600 0.17394600 2.75633000H -1.30732200 -1.52984400 2.22687000H -0.36414500 -1.03785100 3.63534300C 1.44207900 0.56768700 2.40993100H 2.50470200 0.59337300 2.18653700H 1.02120200 1.39027200 2.97677900C -0.58014100 1.20375700 0.09489900O -0.74529000 2.01129400 0.98309200O -1.05655600 1.34265400 -1.14967100C -1.69822400 2.60004600 -1.44138400H -0.98622600 3.41794000 -1.30622100H -2.01149200 2.52652500 -2.48270000H -2.55943800 2.74989800 -0.78486500 SCF energy=-666.1669355C 2.06352000 -1.31269500 -0.21713700O 2.39252500 -2.37232300 -0.73968000C 3.05191700 -0.46942900 0.55860200H 3.02446800 0.58852800 0.28910000H 2.84971800 -0.53738900 1.63270000H 4.04582500 -0.87312000 0.35854300N 0.73303200 -0.92627600 -0.33306800H 0.19669800 -1.64644000 -0.80672500C -1.47474500 -0.32954100 0.49036800O -1.86009800 -0.34332400 1.64729700N -2.18918800 -0.87188500 -0.53669800H -1.92383000 -0.67555600 -1.49177700C -3.50910300 -1.45255300 -0.30057500H -4.24516100 -0.68332700 -0.03959900H -3.82771400 -1.97111300 -1.20756700H -3.45140100 -2.16702400 0.52362500C -0.06151900 0.23680800 0.08882600C -0.19760800 1.33079900 -1.07104300H -0.58176600 0.76836800 -1.93438400C 1.16214000 1.91858300 -1.47811400H 1.60430800 2.49958900 -0.66117000H 1.86489000 1.13553600 -1.77883400H 1.02600900 2.59127300 -2.33123400C -1.17544300 2.39786100 -0.69888600H -2.24189500 2.26837700 -0.85481800H -0.84548100 3.26888300 -0.14086700C 0.48201600 0.89727500 1.28896600N 0.91313800 1.49186600 2.18634200 SCF energy=-805.0116699C 0.02558000 2.53030800 -0.53234200O -0.43753000 3.46312400 -1.18821400C 1.38551700 2.66648000 0.12316200H 1.38683200 3.58999800 0.71079500H 1.68591000 1.82803900 0.74720700H 2.12583300 2.78718000 -0.67487600N -0.71475600 1.36798900 -0.43478500H -1.53886400 1.44070800 -1.02199800C -1.50074200 -0.93812100 -0.50732100O -1.15395500 -2.02913800 -0.93705800N -2.79130300 -0.49706800 -0.62362700H -3.09686500 0.29009600 -0.06687100C -3.82484800 -1.36232400 -1.18432900H -4.04919400 -2.20740600 -0.52200400H -4.72952700 -0.76940200 -1.33899100H -3.48583100 -1.76007300 -2.14331500C -0.49663900 0.04819700 0.20649900C -0.95311700 0.10060200 1.72391700H -1.97076800 0.53248100 1.66800100C -0.18033400 1.08375000 2.62765500H 0.87387000 0.81552000 2.73740400H -0.24394400 2.10779000 2.25060100H -0.63219100 1.07415600 3.62654000C -1.07471800 -1.25192500 2.35501900H -1.16101100 -2.16089000 1.76932800H -1.17775100 -1.32810600 3.43369400C 0.92387100 -0.47841100 -0.05742900C 1.46243600 -0.34536900 -1.34768300C 1.69289200 -1.13152000 0.91216200C 2.73170800 -0.83240200 -1.65381000H 0.87925200 0.14170200 -2.12408700C 2.96973800 -1.61834100 0.61084800H 1.30079100 -1.28278300 1.91217200C 3.49711800 -1.46835200 -0.67122600H 3.12146500 -0.71825400 -2.66219800H 3.54664800 -2.11821700 1.38496600H 4.48887100 -1.84630700 -0.90603500 SCF energy=-897.2844052C -2.50212000 2.26196500 0.00346200O -1.45491700 2.90488100 0.02619400C -3.86086300 2.94253300 0.03790100H -3.95360200 3.58610500 -0.84323300H -4.70406700 2.24411900 0.05908500H -3.91027700 3.58685900 0.92131100N -2.51736000 0.89209300 -0.04167200H -3.40024900 0.43203000 -0.22055400C -1.28459200 0.11693400 -0.24266900H -0.67303700 0.64223000 -0.98000400C -1.61933100 -1.23625400 -0.89126400O -1.04920400 -1.61950700 -1.90503200N -2.63349500 -1.95737200 -0.30993000H -2.87625800 -1.74251000 0.64830600C -2.97310900 -3.28834400 -0.80358900H -2.17807000 -4.01554300 -0.59676600H -3.90002300 -3.61497500 -0.32517500H -3.12085800 -3.24515900 -1.88482000C -0.43306300 0.03394100 1.07590300H -0.32213300 1.08489400 1.36789900C 2.05561600 0.23073600 0.20347000C 3.18676500 -0.62881400 0.19553300C 4.42376900 -0.23467500 -0.31724100C 4.52974400 1.07035600 -0.79859600C 3.42919500 1.95075800 -0.77079600C 2.19120000 1.54572800 -0.27687700C 0.94043700 -0.50285700 0.78805900C 1.44600800 -1.75375900 1.00995900H 5.27608100 -0.90958600 -0.32868400H 5.48159800 1.41577300 -1.19363300H 3.54797100 2.96251300 -1.14967100H 1.34548300 2.22908600 -0.26985800N 2.78864200 -1.84810200 0.76014000H 3.26627500 -2.72321700 0.59461800C -1.11111600 -0.70309500 2.24045800H -2.14021900 -0.35233900 2.38977200H -1.11821300 -1.78992300 2.09128200H -0.56317600 -0.51059300 3.16878200 SCF energy=-957.2366948C -3.22616200 1.87130900 -0.45239500O -2.60742600 2.43689100 -1.35009100C -4.50023400 2.44930000 0.13891600H -5.24026000 2.55350100 -0.66120300H -4.92884700 1.84012200 0.94129600H -4.28825300 3.45156900 0.52440100N -2.81266800 0.67511700 0.07255800H -3.31169400 0.27399700 0.85474800C -1.61672100 -0.00751500 -0.40889500H -1.52717600 0.20779800 -1.47602600C -1.82950900 -1.53330100 -0.28695800O -2.06614700 -2.22158600 -1.27548600N -1.81861200 -2.03072400 0.98240800H -1.38966400 -1.45781500 1.70055600C -1.96416400 -3.46021800 1.22625700H -1.08495900 -4.02141500 0.88498000H -2.10173100 -3.62063900 2.29840400H -2.83757600 -3.83636100 0.68848600C -0.34859200 0.54334600 0.26782300H -0.34294500 1.63019800 0.15121400C 2.27251800 0.42182300 0.08519600C 3.18678900 -0.41324100 -0.61191200C 4.57050900 -0.22996200 -0.55268600C 5.04064200 0.82919900 0.22100600C 4.15271600 1.67385700 0.91850000C 2.77536900 1.47871500 0.86309900C 0.92478500 -0.05687800 -0.19677400C 1.12282000 -1.14014500 -1.00771800H 5.25389900 -0.88191500 -1.09068600H 6.11069900 1.00634000 0.28685100H 4.55338800 2.48936600 1.51465400H 2.10217600 2.12685500 1.41728000N 2.43019800 -1.36955700 -1.29494100H 2.78733700 -2.13263600 -1.85081800F -0.48031600 0.35189200 1.69772800 SCF energy=-1046.5988131C -2.87434700 1.81023300 0.59362600O -2.49790300 2.55402500 -0.31883400C -4.06689800 2.15962600 1.46336500H -4.94869800 2.28017700 0.82574100H -4.27917300 1.41182500 2.23375100H -3.87740100 3.12391800 1.94610000N -2.23873500 0.64017600 0.88392200H -2.66451100 -0.02788900 1.51559200C -1.08112200 0.17967700 0.11446900H -0.54394600 1.08282400 -0.18555000C -1.54102200 -0.56825000 -1.15889300O -1.56425700 -1.79710800 -1.21775600N -1.92930400 0.24736400 -2.16851300H -2.01547000 1.23909100 -1.95887300C -2.50332200 -0.27781300 -3.39893000H -3.51858500 -0.66457300 -3.24223800H -2.53472200 0.52377700 -4.14069300H -1.88188600 -1.09457500 -3.77473500C -0.10550500 -0.67364400 0.97191600H -0.02132000 -0.13834300 1.93101100C 2.24460000 0.31856600 0.30153300C 3.40779300 -0.19535500 -0.33973600C 4.55202200 0.57676300 -0.55300900C 4.53389000 1.89378800 -0.09643200C 3.40099800 2.42194100 0.55495300C 2.25952500 1.64984700 0.75715300C 1.25672700 -0.74805400 0.34810500C 1.86258100 -1.79915000 -0.27485100H 5.42770400 0.16605400 -1.04953700H 5.40927200 2.52096000 -0.24224000H 3.41824600 3.45178200 0.90188900H 1.39455400 2.07806600 1.25823700N 3.14111100 -1.52446600 -0.66453600H 3.72681400 -2.13036300 -1.21969100C -0.63899500 -2.05897400 1.33911300O -0.03691700 -3.10344300 1.29019100O -1.89669300 -1.97929700 1.87627900H -2.17776600 -2.89285600 2.07178800 SCF energy=-1195.114096C -1.72370800 2.73589200 -0.21829700O -0.54841400 3.06766300 -0.06806700C -2.85877000 3.74116100 -0.13804700H -2.69205000 4.51888700 -0.89032600H -3.84927600 3.30106700 -0.29238700H -2.83344300 4.22323800 0.84449000N -2.08485000 1.43739800 -0.45235000H -3.05185400 1.23435100 -0.66604500C -1.09404400 0.38372900 -0.68306000H -0.34880400 0.76305600 -1.38634100C -1.74372600 -0.81909000 -1.39585400O -1.19143200 -1.35671000 -2.34685500N -2.98322800 -1.19789500 -0.94913800H -3.24080800 -0.94132700 -0.00356400C -3.62572000 -2.38782200 -1.50059800H -3.10456700 -3.30538200 -1.20084400H -4.65922000 -2.42288500 -1.14733500H -3.61767200 -2.32902200 -2.59079900C -0.26051600 0.03391000 0.60984700H -0.04987500 1.00627000 1.06606900C 2.30578600 0.09031700 0.02079900C 3.30748300 -0.88445800 -0.23853000C 4.63085400 -0.54349300 -0.52907500C 4.95061200 0.81261600 -0.54951800C 3.97375400 1.79652500 -0.29191800C 2.65409400 1.45306500 -0.01022400C 1.05553800 -0.61268600 0.27825200C 1.37815200 -1.92915900 0.12356300H 5.38235500 -1.30344000 -0.72790500H 5.97112300 1.11548800 -0.76851200H 4.25565600 2.84573700 -0.32183200H 1.90508000 2.22120900 0.16232700N 2.69831700 -2.13694200 -0.14011600H 3.10906900 -3.01872800 -0.40906500C -1.00781800 -0.74775500 1.68612000F -0.35425700 -0.71728600 2.86619200F -2.25594400 -0.23274900 1.92334400F -1.20318200 -2.05558500 1.37289700 SCF energy=-1383.7261127C -2.32366900 -1.53905900 -2.22841600O -1.43964000 -1.24712900 -3.03171100C -3.76714300 -1.74195300 -2.65205600H -3.81314900 -2.59508000 -3.33730600H -4.44916000 -1.92249300 -1.81502700H -4.10224100 -0.85825700 -3.20352700N -2.05772500 -1.69875500 -0.89401300H -2.80460200 -1.95581300 -0.26253400C -0.69252100 -1.64233700 -0.37321500H -0.04299600 -2.13903600 -1.09726300C -0.57132300 -2.50807200 0.90213300O 0.14106700 -3.50798300 0.89901900N -1.33974000 -2.14827000 1.96526700H -1.73246900 -1.21119700 1.97294400C -1.27955700 -2.89693800 3.21408800H -0.30472800 -2.78632800 3.70504400H -2.06398400 -2.52855700 3.87962500H -1.44002300 -3.96010300 3.01739900C -0.16198800 -0.17115400 -0.30722300H -0.09714300 0.14908200 -1.35197500C 2.47320300 0.04783400 -0.42363800C 3.51234100 0.17978300 0.53627600C 4.85864200 0.27652800 0.17722900C 5.15805600 0.26082400 -1.18349200C 4.14171100 0.14710400 -2.15447400C 2.80281700 0.03881700 -1.79027000C 1.21241700 -0.05036300 0.29779600C 1.57754400 -0.01542300 1.61449500H 5.64142100 0.36715900 0.92584100H 6.19406900 0.34099300 -1.50117200H 4.41096100 0.13773400 -3.20712800H 2.03099700 -0.06054900 -2.54930000N 2.91297000 0.17533800 1.79998100H 3.39997500 0.05119100 2.67598900C -1.10485000 0.80650000 0.36748200O -1.88935300 0.59893500 1.26024000O -0.93490200 2.06788600 -0.19137800C -1.62192800 3.14810600 0.31704400F -1.23105000 4.21821000 -0.38359400F -1.34510300 3.36224200 1.61204000F -2.94999600 3.01268300 0.18020000 SCF energy=-778.6147749C -3.08405700 0.90530100 0.07954600O -3.92098400 1.21285600 0.92247800C -3.45399600 0.60976000 -1.36378000H -3.03436200 1.36906300 -2.03639300H -3.08292400 -0.36699600 -1.69195300H -4.54168100 0.63546700 -1.44384300N -1.74890700 0.85063400 0.41729300H -1.55851900 1.00438800 1.40282800C -0.52192800 -1.18885400 -0.39091500O -0.77257900 -1.83345100 -1.41207300N -0.16021400 -1.75784900 0.78221600H 0.14933500 -1.13968000 1.52510800C -0.03165900 -3.20037000 0.93093200H 0.82887300 -3.58847200 0.37223700H 0.09330000 -3.43226000 1.99112200H -0.93160700 -3.69577100 0.55626100C -0.64761900 0.35770400 -0.39489300H -0.83029500 0.62081900 -1.43970300C 0.64839200 1.07503400 0.05224600C 1.83263700 0.65339100 -0.76408700H 0.47686600 2.15434100 -0.13467900H 1.67346300 0.44522100 -1.81975500C 3.18596200 0.65362600 -0.22296700O 3.42903100 0.98577600 0.95454600N 4.19066000 0.28918800 -1.07384300H 4.01578500 -0.04850900 -2.00937000H 5.13343000 0.23981900 -0.71083300O 0.80406100 0.87348600 1.45277100H 1.75494800 1.02587100 1.66103800 SCF energy=-758.7351795C -3.12129300 0.87716400 0.08906300O -4.03634900 0.92243000 0.90453100C -3.34225400 1.12957800 -1.39152100H -2.72093900 1.95510700 -1.75951600H -3.10471900 0.23738300 -1.98218500H -4.39304300 1.38605100 -1.53356100N -1.83297200 0.61425900 0.51545200H -1.80307600 0.31255400 1.48470500C -0.50587600 -1.25797600 -0.43095900O -0.86861100 -1.84174000 -1.45444800N 0.01271700 -1.88279500 0.65214400H 0.38231100 -1.28724200 1.39495600C 0.20328900 -3.32533600 0.68718000H 0.98867100 -3.64527200 -0.00864900H 0.48351100 -3.61565200 1.70250700H -0.72409700 -3.83373600 0.40806500C -0.67605400 0.27636000 -0.30559700H -0.87046300 0.62369600 -1.32103600C 0.59044700 1.01887200 0.21568600C 1.76736500 0.68147500 -0.64600100H 0.38004000 2.09722800 0.06225400H 1.55846800 0.43688600 -1.68562600C 3.16315900 0.78453900 -0.22952200O 3.51274200 1.15557600 0.90306400N 4.09463500 0.47070500 -1.18818600H 3.84264700 0.05099700 -2.07161300H 5.06798900 0.45678300 -0.91397500N 0.80772500 0.73206600 1.64601200H 1.78047000 0.94183400 1.88045400H 0.22256000 1.34555300 2.21010300 SCF energy= -802.6275146C 3.18367100 0.58661500 -0.14872300O 4.06696000 0.59998300 -0.99810500C 3.48243200 0.61062900 1.33856200H 3.02603400 1.48087400 1.82762300H 3.10233500 -0.29471900 1.82332900H 4.56496500 0.66716100 1.46118800N 1.85746900 0.57672700 -0.54144000H 1.73406800 0.45912600 -1.54272300C 0.37499800 -1.17119900 0.37772800O 1.08723400 -1.85067400 1.12011600N -0.59601800 -1.68986300 -0.40072700H -1.27025300 -1.08325400 -0.86339300C -0.90158800 -3.11510600 -0.35158600H -1.25291200 -3.41415600 0.64292600H -1.67964600 -3.32318700 -1.08870300H -0.00780000 -3.70014500 -0.58652000C 0.68324400 0.34954000 0.28491100H 0.92529100 0.64546700 1.30883700C -0.43452100 1.31682100 -0.19486600C -1.69840500 1.30933300 0.59430200H 0.00286200 2.32321100 -0.13271500H -1.65168000 1.81353200 1.55765100C -2.96321900 0.69353500 0.18300900O -3.04970300 -0.14696600 -0.72032700N -4.06359100 1.07226100 0.91283600H -4.05434600 1.88358200 1.51484200H -4.96402800 0.72836000 0.60449100F -0.67283400 1.08894700 -1.55944600 SCF energy=-891.9882666C 3.15669500 0.61037800 0.38582200O 4.04541600 1.09082100 -0.30962100C 3.44336900 -0.03140000 1.73255200H 2.95835900 0.51874000 2.54838200H 3.09387500 -1.06969600 1.77300100H 4.52260900 -0.01123200 1.88980800N 1.84731100 0.64190200 -0.04757800H 1.71929900 1.09424400 -0.94754000C 0.25971900 -1.33417700 0.10708900O -0.59731000 -1.95499400 0.73974400N 0.91190000 -1.83903200 -0.95961400H 1.55495900 -1.23412800 -1.45204600C 0.56915900 -3.13509300 -1.53005200H -0.38869800 -3.09331600 -2.06162300H 1.35808300 -3.43281600 -2.22447900H 0.48875300 -3.87758100 -0.73218700C 0.67536900 0.07490700 0.59364400H 0.91349500 -0.07856500 1.64949200C -0.53007900 1.08974100 0.59925900C -1.74222400 0.52151200 1.27079800H -0.18104300 1.93003700 1.21443600H -1.72890000 0.44309300 2.35433800C -2.85718800 -0.03256800 0.51057400O -2.89955800 0.02749000 -0.72374000N -3.88312900 -0.58297500 1.24867400H -3.69413300 -0.92222000 2.18280200H -4.55904100 -1.11872800 0.71801500C -0.87818000 1.74702100 -0.74374800O -1.52096400 2.76566200 -0.83054900O -0.29645000 1.14976000 -1.81926300H -0.61910400 1.62106400 -2.61098600 SCF energy=-931.295654C 3.20303700 -0.44688700 -0.62987100O 4.03129900 -1.20837600 -0.14082900C 3.58722300 0.62370500 -1.63725900H 3.11178100 0.44589300 -2.60975700H 3.29701300 1.62548100 -1.29959700H 4.66997900 0.58945900 -1.76530500N 1.87603000 -0.54432400 -0.26796700H 1.67751800 -1.29002900 0.39198400C 0.37881800 1.42434400 0.28960400O -0.45010300 2.26563600 -0.06456300N 1.03102100 1.47505500 1.46934400H 1.65441000 0.71366000 1.70052300C 0.72903900 2.48666700 2.47322300H -0.25727800 2.31852000 2.92097500H 1.49369900 2.44637400 3.25223300H 0.73261300 3.47827700 2.01292500C 0.76302300 0.28756900 -0.68658300H 1.06502700 0.81809700 -1.59360800C -0.47630100 -0.58260400 -1.12040500C -1.63552300 0.26417800 -1.54815100H -0.13226200 -1.13293400 -2.00646100H -1.55561300 0.77762100 -2.50248500C -2.78845300 0.51324300 -0.69002500O -2.93529600 -0.04933100 0.40159300N -3.73744600 1.38093700 -1.19115600H -3.45869200 2.07310400 -1.87447100H -4.43541900 1.68626900 -0.52390100C -0.90624400 -1.68877900 -0.14446800O -1.54990900 -2.65008800 -0.49720200O -0.41798100 -1.52262900 1.10510700C -0.91756300 -2.45185500 2.09156400H -0.42779000 -2.17348000 3.02509900H -2.00111500 -2.33946700 2.17113800H -0.66752900 -3.47770800 1.81053900 SCF energy=-795.6195012C -3.21294000 0.56984400 -0.05234000O -4.12199300 0.66738000 0.76116300C -3.46288800 0.47440500 -1.54534700H -2.93310500 1.25875700 -2.10064800H -3.13495700 -0.49927300 -1.92473000H -4.53495600 0.58834000 -1.71193100N -1.89828100 0.57058800 0.38982800H -1.82652100 0.51464300 1.40296900C -0.41538800 -1.29329800 -0.24436200O -1.20553300 -2.05746900 -0.80093500N 0.62647900 -1.71267600 0.50041800H 1.35339800 -1.06658700 0.80195400C 0.89709400 -3.13811400 0.65672000H 1.16364700 -3.60048400 -0.30087000H 1.72439300 -3.25349900 1.35960300H 0.01099800 -3.64680300 1.04615100C -0.71290800 0.22782800 -0.37104300H -0.94067000 0.37328400 -1.42866200C 0.42801900 1.28189000 -0.04069500C 1.63237200 1.18411600 -0.92625000H -0.05918300 2.23854800 -0.27919700H 1.50892200 1.54728600 -1.94413200C 2.91154000 0.59942800 -0.52593700O 3.03402000 -0.07355500 0.50717400N 3.96101500 0.80001600 -1.38192500H 3.92176400 1.47250000 -2.13476700H 4.87180700 0.46569100 -1.09446500C 0.70907600 1.34927100 1.40405800N 0.82202300 1.45414600 2.55463500 |  SCF energy=-972.808371C -2.57932900 -0.45509400 -0.36575100O -2.63467100 -0.02908600 -1.51699500C -3.79166300 -1.05862800 0.32368300H -4.08798200 -1.96412400 -0.21678700H -3.61785100 -1.31233700 1.37422200H -4.62365100 -0.35076600 0.25813200N -1.43530800 -0.40407300 0.38911900H -1.38887200 -0.93857100 1.25056400C 0.82211400 -1.19720200 0.22316300O 0.70990300 -1.76581500 1.31275200N 1.75185600 -1.54918400 -0.69618000H 1.85875100 -0.95949800 -1.51169200C 2.75803500 -2.56794600 -0.42647900H 2.28039300 -3.43945000 0.02721800H 3.22376400 -2.85986600 -1.37058800H 3.53166600 -2.20356600 0.26122100C -0.13864900 -0.05815600 -0.17819500C 0.33880500 1.36899100 0.27854300C -0.66648300 2.42123300 -0.22141500H -0.78120500 2.39077800 -1.30979400H -1.65037900 2.23607800 0.21997700H -0.33878800 3.42405800 0.07134100C 0.51345900 1.47501100 1.79910300H 1.24035000 0.75408300 2.18595300H 0.84177000 2.48336300 2.06978300H -0.44446000 1.28222100 2.29726300S 1.94319600 1.80275600 -0.58597800H 2.77288400 1.10518000 0.22070000H -0.26295400 -0.02892800 -1.26439400 SCF energy=-1177.0108343C -1.74660900 2.59256400 0.09417700O -1.96523700 3.48144900 0.91102000C -1.83627200 2.81344200 -1.40326100H -0.85826800 2.67528100 -1.88090200H -2.53870800 2.11631100 -1.87260800H -2.16838000 3.83873200 -1.57198700N -1.37846900 1.33562500 0.53604200H -1.40136600 1.25936500 1.54853600C -2.57449700 -0.62049000 -0.37752800O -3.20346800 -0.59086500 -1.43029100N -3.04051900 -1.26179600 0.73453500H -2.55920500 -1.13070700 1.61405300C -4.38463500 -1.83048100 0.77576600H -4.54794800 -2.43989300 -0.11581800H -4.47360600 -2.45885100 1.66520100H -5.15302100 -1.04841500 0.80324500C -1.21555900 0.10972500 -0.24508000H -0.94894700 0.38343700 -1.26725400C -0.05950600 -0.74088000 0.34077100H -0.27351700 -0.97435800 1.39404500C 1.28451500 0.00723800 0.26353500C 2.40229100 -0.61809800 1.11769300H 1.11839700 1.03803200 0.59966000H 1.61673500 0.06065400 -0.78123800H 2.08808400 -0.67206000 2.16761800H 2.59444100 -1.64522100 0.80023200N 3.65787900 0.13670500 1.08910300H 3.62156200 1.00661700 1.60834300C 4.44098600 0.24664900 -0.06528900N 4.44786100 -0.90112300 -0.85794800H 5.13161400 -0.81877600 -1.60265400H 4.53327200 -1.77895200 -0.35646400N 5.12450800 1.27202300 -0.43560300H 4.93035700 2.08835000 0.14641500S 0.13418700 -2.34797800 -0.56281400H -1.05196000 -2.88463200 -0.20684200 SCF energy=-1082.7690597C 2.76059000 0.39532000 -0.12438900O 3.69491000 0.45579800 -0.91464100C 2.95038300 0.44180700 1.37851800H 2.39791500 1.27681600 1.82626800H 2.60056800 -0.48586600 1.84387400H 4.01510000 0.57238300 1.57698300N 1.46543000 0.30959700 -0.61052200H 1.43738000 0.21061300 -1.62109900C 0.04930000 -1.53985300 0.20131600O 0.66302600 -2.19332700 1.03782400N -0.77079700 -2.12115800 -0.71594600H -1.22511300 -1.56270200 -1.42345300C -0.94348800 -3.57020700 -0.76099100H -1.28215200 -3.93940200 0.21121900H -1.69087800 -3.80871300 -1.52093100H 0.00002500 -4.06827900 -1.00794400C 0.25584100 -0.00156500 0.13468300H 0.40170000 0.29991200 1.17250600C -0.93981900 0.79928000 -0.41663000H -1.18941700 0.50891800 -1.44255300C -2.16448700 0.62068700 0.46613500O -2.15127600 0.36075300 1.64682100O -3.30863900 0.80723000 -0.24199100H -4.05599600 0.71640700 0.38018000S -0.47163400 2.60012600 -0.46678700H -1.71950100 3.04237400 -0.73713900 SCF energy=-972.7999022C 2.41463900 1.23706000 0.25601200O 3.38909900 1.76458000 -0.27184900C 2.32340000 1.00953200 1.75402500H 1.57137900 1.67241100 2.19995500H 2.04436800 -0.02039200 2.00274600H 3.29569200 1.23944700 2.19205200N 1.34889600 0.82130500 -0.51385100H 1.43575700 1.08807100 -1.48939200C 0.15720100 -1.29331100 0.09786900O -0.64957900 -1.89090800 0.81386900N 1.12756000 -1.93097200 -0.60177700H 1.83404100 -1.36147700 -1.04906000C 1.32553400 -3.37134500 -0.50667200H 0.36687300 -3.88303000 -0.62158900H 2.00315900 -3.68610200 -1.30370200H 1.75070500 -3.65602100 0.46345100C 0.08333700 0.24314000 -0.06730500H -0.16204300 0.63305000 0.92518300C -1.05434600 0.68256400 -1.03817300H -0.76289100 0.34053800 -2.04612700C -1.19143600 2.21439300 -1.06700500H -1.51852700 2.59044600 -0.09138200H -0.25273000 2.71313800 -1.32663700H -1.94203800 2.50973300 -1.80956000C -2.41484000 0.00991900 -0.75818600H -2.35889400 -1.07271700 -0.88374500H -3.13686300 0.38788000 -1.48930700S -3.17585000 0.34327800 0.88949500H -2.46666300 -0.60083300 1.54503900 SCF energy=-1067.483014C 1.57249100 2.17796000 -0.45455800O 1.64828500 3.01600900 -1.34862800C 1.88373800 2.50634800 0.99458800H 0.98560100 2.42229000 1.61788200H 2.64238500 1.83446700 1.41253500H 2.25025400 3.53305700 1.03484100N 1.20869300 0.88068800 -0.75302400H 0.95039200 0.75825900 -1.72822000C 2.09667700 -1.27777700 0.20979200O 1.98885600 -2.27493100 0.92275500N 3.18990000 -1.02483400 -0.55063300H 3.21497700 -0.16037600 -1.07443700C 4.34665700 -1.90961700 -0.55164900H 4.02851400 -2.94178000 -0.72346400H 5.02408600 -1.60064600 -1.35101900H 4.87720400 -1.87178500 0.40691800C 0.95765000 -0.23261200 0.15700400H 0.87733300 0.16588700 1.17224000C -0.37022600 -0.93619800 -0.17859600C -1.63823000 -0.08816700 0.02283000H -0.42549000 -1.84786800 0.42569600H -0.34065900 -1.26267600 -1.22985200C -2.88412900 -0.82665500 -0.49513700C -4.14629700 0.03360100 -0.60576000H -2.66395300 -1.22751100 -1.49417600H -3.08291800 -1.69639900 0.14906100H -4.38104200 0.47745200 0.37361500H -3.95400400 0.86344200 -1.29858200N -5.24501900 -0.76427500 -1.17184600H -5.54735700 -1.47653300 -0.50806000H -6.05523000 -0.17598200 -1.35666600H -1.53234900 0.85694800 -0.52586000S -1.82179400 0.48987200 1.78107800H -1.80116200 -0.73916500 2.34470500 SCF energy= -1122.1022075C 3.19690000 1.16576200 -0.12383100O 4.03581500 1.59537200 -0.90839800C 3.51131700 0.89009900 1.33549800H 3.00193800 1.61375600 1.98433800H 3.19776900 -0.11276700 1.64564700H 4.58815300 0.99402600 1.47573000N 1.90957900 0.91142200 -0.55328700H 1.73985100 1.20683800 -1.50986100C 0.66143000 -1.05852100 0.41501200O -0.08461400 -1.51667300 1.28360200N 1.41325800 -1.82093700 -0.40791800H 1.97471000 -1.34979200 -1.10521700C 1.33362200 -3.27526400 -0.41169300H 0.45438900 -3.62286100 -0.96691200H 2.23760900 -3.67929900 -0.87388100H 1.25846700 -3.63549800 0.61693600C 0.76728700 0.47227200 0.24205900H 0.86500300 0.86370800 1.26004200C -0.51216400 1.08646100 -0.38019800C -1.83040600 0.69323500 0.30039200H -0.57432700 0.81109100 -1.43948800H -0.38861400 2.17359500 -0.32427500H -1.71763400 0.62715000 1.38383200C -2.37915200 -0.62825300 -0.21714700O -2.04644300 -1.17632000 -1.24683200O -3.34140000 -1.11373000 0.59887500H -3.65332500 -1.95443400 0.21452700S -3.07342000 2.03301100 -0.06847200H -4.06899400 1.51897600 0.68403000 SCF energy=-1012.102875C -1.90746500 -2.14138600 -0.03965500O -2.60586300 -2.73810100 -0.85354600C -1.56089700 -2.73488500 1.31438600H -0.48894300 -2.68547800 1.53160800H -2.09168400 -2.20369800 2.11444700H -1.88135100 -3.77767500 1.31674400N -1.41774000 -0.88763700 -0.33850200H -1.80813300 -0.51978600 -1.19923600C -0.68600700 0.02778600 0.54082300H -0.95763100 -0.19777300 1.57402400C 0.87407900 -0.12335200 0.45288600C -1.20286700 1.46939500 0.34632100O -1.63263800 2.11898100 1.29412600N -1.19015600 1.96641000 -0.92642500H -0.67096100 1.47928500 -1.64379400C -1.64000100 3.32508900 -1.21319300H -0.94141200 4.07379500 -0.82083700H -1.72982100 3.44310100 -2.29566900H -2.61492800 3.49151500 -0.74934900H 1.07287700 -1.14729900 0.79751800C 1.54462200 0.85869900 1.43714600H 0.99071600 0.82266300 2.38456000H 1.42202000 1.88493400 1.06308400C 1.39614200 -0.02919700 -0.99464600H 0.66345200 -0.47546800 -1.67303700H 1.56671300 1.01403400 -1.28159000S 2.97424700 -0.97302500 -1.25682400H 2.72532100 -1.33002700 -2.53479400C 3.02903100 0.59713700 1.72640700H 3.19295800 -0.42736900 2.08284900H 3.66021800 0.74866300 0.84421400H 3.38610500 1.28082600 2.50544600 SCF energy= -1067.4819195C 2.20108100 2.13341000 -0.00482900O 2.43121500 3.06593700 -0.76852000C 2.62178600 2.15883500 1.45438900H 1.74581500 2.23731100 2.11026300H 3.17582800 1.25875400 1.74339500H 3.25107100 3.03664100 1.60798500N 1.54777600 1.00737900 -0.46023800H 1.22062800 1.09766300 -1.41770600C 2.11908100 -1.35638700 0.22254600O 1.90646200 -2.37655300 0.87686700N 3.19607900 -1.20238700 -0.58506900H 3.31797000 -0.31259100 -1.04963300C 4.21196100 -2.23742200 -0.71895300H 3.74107300 -3.19799300 -0.94645400H 4.88751400 -1.96248600 -1.53213400H 4.78774200 -2.35116800 0.20685900C 1.12515100 -0.17114300 0.29053500H 1.06433200 0.09367100 1.35117900C -0.27147200 -0.64659500 -0.16129700C -1.38983100 0.35315500 0.17338200H -0.44556900 -1.61248800 0.32043400H -0.24830300 -0.83405000 -1.24616600C -2.78076700 -0.08802800 -0.31554600H -1.42943800 0.51701500 1.25964500H -2.70463900 -0.39771700 -1.36714300H -1.15038300 1.32495900 -0.27597100C -3.36462400 -1.25074000 0.50115100H -2.62458800 -2.06711000 0.53451300H -3.52455200 -0.90995800 1.53063100N -4.66103600 -1.68313900 -0.03732100H -4.54065300 -2.22651300 -0.89063700H -5.15307300 -2.27568700 0.62703700S -3.90311600 1.38658900 -0.25798100H -5.03625400 0.65776400 -0.37505200 SCF energy=-1239.8108125C 0.23872300 1.96193900 1.37655500O -0.31365100 3.02830100 1.12378000C 0.45234900 1.48416000 2.80172000H -0.17876100 0.61401400 3.01705300H 1.49370400 1.20150700 2.99405800H 0.16979800 2.29628600 3.47325700N 0.72404700 1.17722600 0.34779700H 0.39390600 1.49005700 -0.56270000C 2.59216400 -0.36321000 -0.18740100O 3.05950000 -1.45789700 -0.51061700N 3.30523900 0.78164400 -0.29817300H 2.84389000 1.64953000 -0.06046400C 4.66834400 0.78628500 -0.81031200H 4.69818800 0.43664900 -1.84803200H 5.05565100 1.80637700 -0.76082300H 5.30444900 0.12670800 -0.21179900C 1.16495500 -0.21385900 0.40964400H 1.23899800 -0.50222500 1.46206400C 0.14839700 -1.19305700 -0.27999300H 0.33633800 -1.16959200 -1.35499300S 0.39382900 -2.95099500 0.26945400H 1.70028200 -2.97450400 -0.07391200C -1.29868800 -0.78933800 -0.04025500C -1.93552200 0.08430600 -0.95046700C -2.03976000 -1.24481400 1.05487500C -3.27181600 0.45564800 -0.77377500C -3.37387300 -0.87186500 1.24676500H -1.56833300 -1.91902100 1.76453500C -3.98753800 -0.02567000 0.32629700H -3.75730600 1.12582700 -1.47374000H -3.92443900 -1.24788900 2.10438200H -5.02457000 0.27204200 0.45723600O -1.15332300 0.54967200 -1.98250700C -1.75312600 1.36598000 -2.98595500H -2.11158200 2.31275100 -2.56384700H -0.96441000 1.56556300 -3.71348300H -2.57992900 0.84013000 -3.47886900 SCF energy= -1259.2506399 C -0.65394600 2.26027200 -1.06081100O -0.07641700 3.28514500 -0.70656800C -1.29503200 2.12741600 -2.43043700H -0.68742100 1.47890900 -3.07402100H -2.30312600 1.70087900 -2.38307100H -1.33939300 3.11931600 -2.88288800N -0.75536800 1.18923500 -0.19995100H -0.17246000 1.27823800 0.63336200C -2.65610800 -0.41969400 -0.04728400O -3.27910900 -1.42727600 -0.39516800N -3.19356800 0.52079400 0.76304800H -2.65622100 1.36322000 0.92179300C -4.56048400 0.41958400 1.25467300H -4.71698800 -0.55216200 1.73124200H -4.72861500 1.21372100 1.98556100H -5.28502300 0.51895400 0.43808600C -1.19813900 -0.16969200 -0.51130000H -1.18505700 -0.33434400 -1.59211400C -0.17802200 -1.16013300 0.15034600H -0.27080600 -1.01721200 1.22684300S -0.50013600 -2.95650600 -0.19441700H -1.84945900 -2.86557100 -0.18004400C 1.25012000 -0.82434800 -0.28213300C 2.09286300 -0.02142200 0.52585500C 1.72240300 -1.24597500 -1.53231900C 3.36805800 0.32328700 0.05518200C 2.99132900 -0.89182600 -1.99469700H 1.08080800 -1.86498100 -2.15289900C 3.81699700 -0.10242000 -1.19599300H 4.01746900 0.93974100 0.66826500H 3.32658500 -1.23111100 -2.97113700H 4.80821300 0.18314500 -1.53904900N 1.60527800 0.46358200 1.79101400C 2.11647300 1.77095300 2.21230200H 1.51210200 2.12131300 3.05647200H 3.16860800 1.74406800 2.54608200H 2.01870500 2.49117500 1.39535700C 1.72539100 -0.52114600 2.87709400H 2.77646200 -0.66521000 3.18323800H 1.15535300 -0.17393900 3.74621900H 1.33084500 -1.49142800 2.56561300 SCF energy=-1353.1892462C -0.65042500 -1.59719900 -2.03722600O -0.21102200 -1.36150300 -3.15817300C -1.00916000 -3.00623100 -1.59572900H -0.31542400 -3.36233600 -0.82498000H -2.02504800 -3.07042000 -1.18915600H -0.92873800 -3.65924500 -2.46599300N -0.86687700 -0.56288700 -1.14859100H -0.48648000 0.32590800 -1.46617600C -2.55632000 0.05462900 0.56787200O -2.89164600 0.37209800 1.71111700N -3.35995800 0.25837100 -0.50160600H -2.99823400 0.02235000 -1.41587200C -4.68024400 0.85781700 -0.36391300H -4.60830100 1.88160600 0.01907400H -5.16090100 0.87081100 -1.34453500H -5.29291000 0.27775800 0.33317600C -1.19942400 -0.64234800 0.26895200H -1.33355200 -1.69621200 0.52816000C -0.06527200 -0.06757600 1.18895000H -0.20634800 1.00743300 1.26578400S -0.17490500 -0.73184800 2.92584200H -1.43484000 -0.28386800 3.11943600C 1.32966200 -0.36391000 0.65228600C 2.14441300 0.61641500 0.03834900C 1.86141900 -1.65431300 0.80269500C 3.45330700 0.29343300 -0.36081500C 3.14818500 -1.97580200 0.37212900H 1.26131600 -2.41608300 1.29261900C 3.95481600 -0.99477800 -0.20746100H 4.06392900 1.07449300 -0.80219000H 3.52255800 -2.98768500 0.50373100H 4.96356300 -1.22929200 -0.53533300C 1.74401000 2.03009100 -0.24994700O 2.51070600 2.97144500 -0.23908400O 0.43436200 2.16813800 -0.59863400C 0.01300300 3.51416200 -0.91380300H 0.17798800 4.17160400 -0.05710000H 0.57067900 3.88968300 -1.77493300H -1.04996800 3.43690600 -1.14363300 SCF energy=-1329.8036493C 0.65595700 2.50503900 -0.33498900O 0.18167600 3.18461200 -1.23922500C 1.06690400 3.11441400 0.99537700H 0.40632500 2.77855300 1.80374400H 2.09488000 2.85411000 1.27255000H 0.98249300 4.19841000 0.90557700N 0.86236500 1.15243800 -0.52032100H 0.47176400 0.79390000 -1.38964500C 2.57279200 -0.52814200 0.17288700O 2.94826300 -1.52846200 0.79012600N 3.32587900 0.06201000 -0.78006600H 2.92201500 0.83875800 -1.28647200C 4.62216700 -0.47377600 -1.17438000H 4.51267800 -1.43855500 -1.68229800H 5.10269000 0.23782500 -1.84924600H 5.25114100 -0.62117400 -0.29209100C 1.21045700 0.15332200 0.48123400H 1.33372100 0.66043000 1.44185600C 0.08804600 -0.93283100 0.66156300H 0.24131000 -1.70433600 -0.09023000S 0.19416800 -1.78040800 2.31597800H 1.48244800 -2.15020600 2.13596700C -1.31095800 -0.34809200 0.51964800C -2.12290100 -0.51896500 -0.61816900C -1.88594300 0.37001200 1.58018500C -3.43279900 -0.03789500 -0.69559000C -3.17838500 0.88996000 1.50885300H -1.30884900 0.50248800 2.49040800C -3.96033300 0.68324600 0.37000100H -4.01056200 -0.22204400 -1.59425000H -3.57762400 1.44827800 2.35110400H -4.96971900 1.07876900 0.31004800N -1.62879500 -1.20390500 -1.82506700O -2.41782800 -1.90340800 -2.45305700O -0.45055700 -1.01527000 -2.16087000 SCF energy= -1651.015961C -0.54171100 -1.89699600 -2.20239600O -0.16363400 -1.49004300 -3.29548500C -0.78515000 -3.37218900 -1.93284300H -0.05084300 -3.76955600 -1.22233800H -1.78434000 -3.56034600 -1.52359100H -0.67872400 -3.90538800 -2.87863500N -0.79438500 -1.00037000 -1.18199000H -0.52234600 -0.04902100 -1.41408300C -2.46755000 -0.74385500 0.64751100O -2.77397000 -0.60773700 1.83403700N -3.32928700 -0.47898200 -0.35955400H -2.97893600 -0.52710100 -1.30687300C -4.67166900 0.02732500 -0.10412500H -4.63877400 1.03522300 0.32449800H -5.21952200 0.05312200 -1.04851900H -5.19180700 -0.62744500 0.60057000C -1.07102900 -1.27912200 0.22157800H -1.10943100 -2.36438000 0.34774600C 0.04192500 -0.72939100 1.18289200H -0.19299300 0.30566900 1.41622400S 0.06012900 -1.62757000 2.81481600H -1.22355200 -1.31773100 3.10287200C 1.43974000 -0.82527800 0.58453000C 2.18908600 0.29808300 0.15924600C 2.05713900 -2.08260500 0.50030600C 3.51524000 0.14071500 -0.28672800C 3.35761100 -2.23689700 0.02163700H 1.51396100 -2.95710100 0.84700300C 4.09741700 -1.11866800 -0.36796400H 4.07159600 1.02496000 -0.58036900H 3.79636800 -3.22976300 -0.03119400H 5.11578000 -1.22559800 -0.72977300C 1.71665300 1.70802400 0.13239600O 2.38577400 2.68749000 0.31491300O 0.35226700 1.79956800 -0.23090300C -0.25005900 3.03735600 -0.29263200F 0.29426000 3.82634700 -1.22620500F -0.22407000 3.67454800 0.88416900F -1.53376200 2.81441700 -0.62582200 SCF energy=-1048.0578109C -2.56085700 -0.57793100 -0.15120900O -2.76780100 -0.12009900 -1.28596300C -3.68356000 -1.19857800 0.65633400H -4.07187600 -2.06420500 0.10949300H -3.37789000 -1.51549100 1.65789000H -4.49772500 -0.47192100 0.74136800N -1.33764000 -0.55594300 0.43711200H -1.20267900 -1.00473400 1.33711100C 0.99019300 -1.09421200 0.34094300O 1.01865900 -1.38328700 1.54263900N 1.80548100 -1.60260100 -0.59667500H 1.65698500 -1.27297300 -1.54331900C 2.89636100 -2.51556900 -0.30147800H 2.75423400 -2.91107600 0.70571700H 2.89667600 -3.34167500 -1.01973600H 3.86520600 -2.00263600 -0.34901000C -0.08016800 -0.09266200 -0.18664000C 0.24060200 1.39741800 0.26014300C -0.70202400 2.37624100 -0.46241300H -0.57216100 2.34638400 -1.54772100H -1.74717400 2.13895100 -0.23975000H -0.50012300 3.39579600 -0.11956100C 0.13329500 1.60239600 1.78009000H 0.77519700 0.91549600 2.33743800H 0.41550900 2.63034600 2.02766600H -0.90049700 1.44816400 2.11224400S 1.96047100 1.86264400 -0.30977000H 2.62931100 1.31338300 0.72826800O -0.13765300 -0.20130200 -1.58472300H -1.07411700 -0.04141100 -1.85508900 SCF energy=-1012.1215426C -2.64719500 -0.39532600 -0.16253700O -2.96901000 0.49206300 -0.94951000C -3.69767700 -1.31647100 0.44699600H -4.13263400 -1.92597400 -0.35296100H -3.30897200 -1.98090800 1.22500900H -4.50180800 -0.70323300 0.86485300N -1.36690100 -0.64118900 0.25849700H -1.21192500 -1.49441700 0.79200500C 0.91544500 -1.28122800 0.03580500O 0.55507400 -2.28471200 0.66025400N 2.17720800 -1.14756800 -0.42535600H 2.47055200 -0.23458500 -0.75813400C 3.19457500 -2.14991100 -0.13435800H 2.84742100 -3.13694000 -0.45079500H 4.10135400 -1.89202700 -0.68633900H 3.42200600 -2.19666000 0.93779100C -0.10370500 -0.12287500 -0.28708500C 0.28927800 1.21655800 0.48910700C -0.86862500 2.22920300 0.51470400H -1.23320800 2.47090700 -0.48472700H -1.70946200 1.83657300 1.09422800H -0.52678600 3.15460400 0.99046600C 0.71804500 0.90469700 1.93266200H 1.62867200 0.29989300 1.98438700H 0.89083900 1.83342500 2.48804400H -0.08385600 0.35834400 2.44220700S 1.72608300 2.05456800 -0.42330300H 2.34127500 2.52205200 0.68263200C -0.18819800 0.05432100 -1.81964000H 0.78264800 0.31871500 -2.24579900H -0.50529200 -0.88984600 -2.27468400H -0.92047200 0.81567800 -2.08719700 SCF energy=-1028.1761225C -2.59652200 -0.51076700 -0.22905400O -2.85290400 0.24524200 -1.16871700C -3.68922400 -1.34546500 0.42295900H -4.10398700 -2.02748400 -0.32718700H -3.34606100 -1.92852500 1.28320500H -4.49723000 -0.67863500 0.73996000N -1.35013800 -0.66572800 0.30600700H -1.20470300 -1.37024700 1.02418700C 0.97143200 -1.20774500 0.19723200O 0.76797800 -1.93229900 1.17649200N 2.05887700 -1.30416100 -0.59007400H 2.16953400 -0.59546500 -1.30578300C 3.16870700 -2.19232900 -0.27847200H 2.77890900 -3.13516500 0.11106100H 3.73737200 -2.38236700 -1.19214200H 3.83538500 -1.75403900 0.47514200C -0.08089000 -0.12378600 -0.22378300C 0.23714500 1.27703600 0.46007200C -0.94365600 2.25647000 0.32669300H -1.23968100 2.42325800 -0.71080500H -1.81688100 1.89270900 0.87807600H -0.65242200 3.22335700 0.75030100C 0.58478300 1.11006300 1.94827800H 1.49828100 0.53086400 2.10454000H 0.71535000 2.09449900 2.41128800H -0.23241300 0.60262800 2.47350200S 1.70802400 2.01077000 -0.46006300H 2.16095400 2.72614900 0.59379500N -0.04348900 0.02449800 -1.66896500H -0.20324900 -0.87895800 -2.11367900H -0.81554200 0.61843600 -1.96899000 SCF energy=-1072.0714236C -2.60329500 -0.55492700 -0.17728700O -2.92406200 0.21110200 -1.07379100C -3.61134500 -1.48449500 0.48594100H -3.74273700 -2.37116100 -0.14589500H -3.31136500 -1.81580900 1.48577100H -4.57327700 -0.96995300 0.54526700N -1.31865100 -0.69154800 0.30918100H -1.16003900 -1.35855700 1.05710700C 1.01953600 -1.10377100 0.28744500O 0.99617200 -1.53890300 1.44195600N 1.91946400 -1.45836200 -0.64584000H 1.87476000 -0.98633200 -1.53956600C 3.04166500 -2.33898100 -0.35753400H 2.75615700 -3.02294400 0.44363100H 3.29069300 -2.91061700 -1.25541700H 3.92448700 -1.77140100 -0.03662600C -0.08558900 -0.10860800 -0.18184700C 0.17321700 1.36946300 0.29530900C -0.75296100 2.35997300 -0.43383200H -0.59850800 2.34274000 -1.51570500H -1.80059800 2.11245100 -0.25294000H -0.55227100 3.37063300 -0.06435700C -0.00362000 1.49370600 1.81638500H 0.63928000 0.80224800 2.36846300H 0.23204300 2.51692100 2.12347000H -1.04308400 1.28296800 2.09190000S 1.90629300 1.89940200 -0.18173200H 2.55622600 1.30027600 0.84116400F -0.09340700 -0.11491900 -1.58163900 SCF energy=-1086.1453689C -2.62328300 -0.45293800 -0.14542100O -2.77798900 0.33984100 -1.07350300C -3.78769100 -1.21320300 0.46294200H -4.29425800 -1.77284600 -0.32971600H -3.49279800 -1.90270700 1.25973300H -4.50659300 -0.49128300 0.86441100N -1.40033600 -0.69126700 0.41665000H -1.27693000 -1.48998600 1.03499300C 0.88642400 -1.32829500 0.17214900O 0.57663700 -2.26792400 0.90799800N 2.06386300 -1.25788100 -0.47888000H 2.31946500 -0.36381900 -0.88925800C 3.11037100 -2.25088600 -0.26571500H 2.68015700 -3.25290200 -0.32687100H 3.86552500 -2.13037300 -1.04552700H 3.58231000 -2.13755300 0.71814200C -0.14008100 -0.15621500 -0.09247600C 0.25759700 1.18040600 0.66924600C -0.83957200 2.24952600 0.51230100H -1.01355100 2.50560600 -0.53409200H -1.78379600 1.90116700 0.94208100H -0.53243900 3.15516600 1.04459500C 0.47545700 0.88385400 2.16235500H 1.29427600 0.17876000 2.33978800H 0.69682500 1.81310700 2.69788200H -0.43616400 0.45835500 2.59629700S 1.84539500 1.92061300 -0.04271100H 2.52683500 1.92482000 1.12555700C -0.24917100 0.00476700 -1.62615000O 0.25199500 0.91085700 -2.25263100H -0.74531600 -0.84558000 -2.12932600 SCF energy= -1177.3412719 C 2.60705700 -0.28023300 -0.15157600O 2.81480100 0.56724800 0.70374700C 3.70805700 -1.13755700 -0.74762600H 3.81970600 -2.04297400 -0.13821300H 3.49981700 -1.44093600 -1.77890300H 4.64757400 -0.58245500 -0.70809600N 1.34486200 -0.55274700 -0.64949700H 1.21860800 -1.42367400 -1.16668900C -0.91563700 -1.28187700 -0.40293400O -0.57131600 -2.18353000 -1.16657800N -2.10734700 -1.23979100 0.21136200H -2.37598400 -0.37978100 0.68296800C -3.10452600 -2.28363100 0.00101300H -2.65483300 -3.26458400 0.17434100H -3.91954300 -2.12741900 0.71047400H -3.49989900 -2.25970700 -1.02104500C 0.10396600 -0.10986500 -0.07832800C -0.35048800 1.30243800 -0.62507300C 0.73152100 2.38479100 -0.45455400H 0.99410300 2.54388200 0.59137400H 1.63995400 2.11424600 -0.99890200H 0.34753400 3.32303800 -0.86646100C -0.66260900 1.13700200 -2.12674500H -1.48816300 0.44340400 -2.31733300H -0.92338200 2.11025900 -2.55431500H 0.22278500 0.76455000 -2.65209000S -1.90319300 1.93482300 0.24805600H -2.64799800 2.05170200 -0.87425300N 0.25096300 -0.13785700 1.49343900O -0.14030500 0.82963400 2.13286000O 0.70274800 -1.17089900 1.96447900 SCF energy=-1498.5575679C -0.53385000 -2.43825500 -0.59706700O -1.01633900 -2.44596600 0.53214000C -0.89463400 -3.47923600 -1.63959600H -1.94034500 -3.33237900 -1.93227000H -0.26675800 -3.43614100 -2.53458800H -0.81557400 -4.47235200 -1.18789100N 0.36823200 -1.48837800 -0.99857200H 0.56245600 -1.37161600 -1.99187400C 0.96155500 0.80551700 -1.33177900O 1.03488500 0.47899400 -2.51641300N 1.05221800 2.07843100 -0.90574300H 1.18668900 2.23833000 0.08924900C 1.29939400 3.17478500 -1.83593500H 0.62218500 3.08968300 -2.68877300H 1.11248000 4.11678000 -1.31609400H 2.33014500 3.16330800 -2.21044600C 0.71065200 -0.30228100 -0.22505800C 2.01056600 -0.56652500 0.65861100C 1.81879900 -1.76840900 1.60210900H 0.99237100 -1.61864700 2.29812900H 1.62480400 -2.68005300 1.02989300H 2.73783300 -1.91208600 2.17846400C 3.20630900 -0.83668600 -0.27091200H 3.43635300 0.01049200 -0.92535300H 4.09466400 -1.06376100 0.32696200H 2.99725000 -1.70549100 -0.90403300S 2.41434500 0.92092200 1.75387300H 3.62445000 1.17377700 1.20816400C -0.48961000 0.15317500 0.63367700O -0.47045000 0.47042400 1.78808700O -1.60506700 0.29262500 -0.18879500C -2.78215400 0.77400200 0.33408800F -2.65447300 2.03963500 0.77250700F -3.25439800 0.02287700 1.33193700F -3.67535900 0.76747900 -0.66669700 SCF energy= -1048.0342427C 2.78921900 0.36245200 -0.00790000O 3.83476400 -0.07191300 -0.48759600C 2.78134500 1.57681900 0.89601700H 1.98102100 2.27944800 0.65964400H 2.63435400 1.26491300 1.93519600H 3.75566000 2.06012800 0.80060700N 1.61213000 -0.30920000 -0.29267100H 1.79710600 -1.12753900 -0.86386700C -0.36887700 -1.49675000 0.41388000O -0.63449800 -1.75818500 1.58601400N -0.47896400 -2.40037300 -0.58751900H -0.37166100 -2.09353000 -1.54437600C -0.95298000 -3.76088200 -0.34388400H -2.02283300 -3.77407700 -0.10652700H -0.77128600 -4.35920400 -1.23928200H -0.40691600 -4.19317100 0.49775800C 0.19771500 -0.07495700 0.06923200C -0.58276800 0.62169800 -1.08551700H -0.45503100 -0.01588100 -1.97581100C -0.00340100 1.99734800 -1.44353900H -0.07804300 2.69205200 -0.60338400H 1.04382000 1.91587700 -1.74908700H -0.56369900 2.42814800 -2.28149700C -2.10663700 0.66928300 -0.84052200H -2.49487200 -0.33346600 -0.63460800H -2.57921900 1.02468600 -1.76079200S -2.63651900 1.80171300 0.53177700H -3.87134600 2.02149200 0.02700300O 0.08508000 0.69419000 1.22642900H -0.14936700 0.06692300 1.94654000 SCF energy=-1087.3294792C -2.31074300 -1.42202500 -0.18030200O -3.51944800 -1.38568600 -0.39789400C -1.62773900 -2.72877400 0.16845000H -1.61772200 -3.36878100 -0.72032900H -0.61224500 -2.61261300 0.54283600H -2.24889000 -3.22979300 0.91707400N -1.59864600 -0.23185200 -0.24308500H -2.24724200 0.54443200 -0.32136100C -0.18997600 1.68232700 0.29565000O 0.40091400 2.17856200 1.24519800N -0.87487800 2.44316400 -0.61060300H -1.18101400 2.02462600 -1.47900600C -0.86499600 3.90115500 -0.52571700H 0.12152400 4.31360000 -0.76924100H -1.60769400 4.29627000 -1.22260800H -1.12307600 4.20886200 0.48999200C -0.19468600 0.12668700 0.04124000C 0.78081400 -0.14518900 -1.16074600H 0.48070400 0.57250900 -1.93843700C 0.67640800 -1.53566600 -1.79658600H 0.96920500 -2.32639300 -1.10395100H -0.33445000 -1.73050400 -2.16561200H 1.35544500 -1.58527100 -2.65657100C 2.23990700 0.23442600 -0.81388400H 2.27755200 1.20879100 -0.32173800H 2.79874700 0.31080000 -1.75049600S 3.14976000 -0.97340100 0.26512100H 4.25526500 -1.04280200 -0.50855200O 0.33598100 -0.56619300 1.13557400C -0.30288300 -0.44524800 2.41432100H 0.18388300 -1.19004200 3.04718300H -0.15397200 0.55315300 2.83016000H -1.37373200 -0.67124000 2.34694400 SCF energy=-1106.7605862C 1.99953000 1.90422500 -0.47145400O 2.71286900 2.33560600 -1.37604800C 1.80265300 2.69808900 0.80196300H 0.78318800 2.64062400 1.18233700H 2.46421500 2.30800700 1.58444500H 2.09204300 3.72975200 0.59181200N 1.44961100 0.63485200 -0.63360500H 1.61435300 0.35549900 -1.59799400C 0.54583500 -1.61554000 -0.19384700O -0.30938300 -2.43747600 0.14011400N 1.76869600 -2.00751600 -0.64167100H 2.49874700 -1.31089300 -0.70266500C 2.13857800 -3.41751900 -0.67313300H 1.36965900 -3.98804100 -1.19952900H 3.08945500 -3.51703000 -1.20182700H 2.23759100 -3.83195600 0.33760100C 0.27439000 -0.06892400 -0.04094700C -0.97991100 0.34588900 -0.93038200H -0.59276100 0.14759000 -1.94016100C -1.26573600 1.85603900 -0.88618600H -0.38031100 2.44356300 -1.13859200H -2.02992500 2.10517900 -1.63087500H -1.63777600 2.18321600 0.08810700C -2.28214200 -0.52974200 -0.87237900H -2.09890700 -1.45554600 -0.32992700H -2.54450500 -0.81830800 -1.89355700S -3.82832700 0.14432800 -0.11684400H -4.14504700 1.02805200 -1.08722100N 0.19581500 0.26045300 1.38150700C -1.07171500 0.01503600 2.06960800H -1.89527900 0.52580800 1.57341300H -1.31403700 -1.05579800 2.15970000H -0.98592200 0.43299300 3.07914200C 1.30639400 -0.26431800 2.18351000H 1.33073100 0.27287000 3.13790700H 1.20277100 -1.34128800 2.40219500H 2.26094600 -0.10250800 1.67853300 SCF energy=-1161.3947359C 2.35901800 1.41649100 -0.46945400O 3.53482200 1.39401700 -0.81886200C 1.71883800 2.71416000 -0.01928700H 0.67025600 2.65088000 0.26703000H 2.29889400 3.08705600 0.83051200H 1.81923300 3.44351200 -0.82928400N 1.64139200 0.22959600 -0.50420800H 2.28560400 -0.54163300 -0.64532400C 0.36038600 -1.68427900 0.30865800O -0.06198100 -2.14580500 1.36095200N 0.89110200 -2.46379500 -0.67412800H 1.06423600 -2.06594900 -1.58779200C 0.93807100 -3.91733300 -0.53767200H -0.06166000 -4.36116900 -0.61124300H 1.57558400 -4.32022700 -1.32783200H 1.35918400 -4.17799300 0.43576900C 0.31300000 -0.14500700 0.00827500C -0.82448700 0.09098300 -1.06566400H -0.50571500 -0.55586800 -1.89498100C -0.88346200 1.50460000 -1.65441200H -1.20267300 2.24725900 -0.92039600H 0.08080500 1.79542800 -2.08032400H -1.61882200 1.52127300 -2.46703600C -2.22178100 -0.45949300 -0.63798100H -2.12354300 -1.19220400 0.16438800H -2.66273200 -0.98287700 -1.49030800S -3.50112400 0.74590900 -0.05199200H -4.22580700 0.75206600 -1.19301900C 0.01240300 0.49485800 1.38014200O -1.06741700 0.91393400 1.72606000O 1.10527900 0.52082200 2.17071400H 0.82013000 0.85166600 3.04353600 SCF energy=-1200.7021071C -2.41451000 0.76735300 1.13737300O -3.51383200 0.46309300 1.59117000C -2.07530300 2.21946900 0.86636200H -1.06794100 2.40942400 0.49913900H -2.79874500 2.59529800 0.13604800H -2.22490300 2.78226200 1.79315600N -1.50126100 -0.24494500 0.89080000H -1.96966300 -1.14158000 0.97055400C -0.04109700 -1.71445700 -0.39885000O 0.27978800 -1.90380300 -1.56551200N -0.26885100 -2.73788100 0.47141600H -0.35830400 -2.54072600 1.45935600C -0.07979500 -4.12734300 0.06320900H 0.98016700 -4.35853000 -0.09475000H -0.48316700 -4.77698500 0.84320200H -0.61410800 -4.30974500 -0.87186700C -0.20730000 -0.26952000 0.18730800C 1.00129400 -0.01298500 1.17478000H 0.88246100 -0.81702000 1.91499700C 0.91789400 1.29104100 1.97539400H 1.02377400 2.17255200 1.33983500H -0.01911300 1.34924800 2.53629300H 1.73804800 1.31891200 2.70179000C 2.40326900 -0.25742300 0.53079600H 2.31519300 -0.85733700 -0.37622500H 3.01155100 -0.83370900 1.23268900S 3.42292700 1.21495000 0.05301200H 4.30148800 1.11845000 1.07578200C -0.18666700 0.64853800 -1.05572700O 0.77024400 1.30870200 -1.39519100O -1.34820100 0.60193300 -1.72160200C -1.38252400 1.31211500 -2.97665300H -0.63202600 0.89954100 -3.65526700H -2.38801800 1.15450600 -3.36643500H -1.18829400 2.37587900 -2.81687000 SCF energy=-1065.0288164C -2.81489000 -0.43993000 -0.16058900O -3.86185900 0.06885300 -0.54687800C -2.78958600 -1.82076800 0.45669600H -1.92540600 -2.42118800 0.17105100H -2.77971100 -1.73405400 1.54882900H -3.70892500 -2.32652100 0.15567200N -1.65363000 0.31657100 -0.28413700H -1.88540300 1.25650600 -0.58867000C 0.30340700 1.55021800 0.49030200O 0.74753000 1.78271700 1.60131000N 0.18963800 2.50438500 -0.47852300H -0.01152300 2.23378400 -1.43164300C 0.65144000 3.87006500 -0.23873500H 1.74501400 3.92096300 -0.18196000H 0.29755600 4.50457700 -1.05426900H 0.24092000 4.23238300 0.70626500C -0.23568600 0.12552000 0.08470500C 0.60146300 -0.44938600 -1.12824300H 0.36851500 0.23977900 -1.95336400C 0.14390900 -1.84019400 -1.58308800H 0.28777300 -2.59432400 -0.80429700H -0.90699800 -1.82853800 -1.88498200H 0.73556800 -2.15235000 -2.45100700C 2.13461400 -0.35235800 -0.95401800H 2.42131800 0.64523400 -0.60883800H 2.57464000 -0.50016300 -1.94433300S 2.89189900 -1.61346200 0.17881400H 4.09556700 -1.60330400 -0.43186200C -0.10205800 -0.73053500 1.27868900N -0.00176900 -1.44177700 2.18874800 SCF energy=-1203.8768107C 1.32679900 2.13515700 1.33230400O 1.46659200 3.35093200 1.45980000C 2.20223200 1.18296900 2.12170900H 2.18899400 1.50327800 3.16799800H 1.92891200 0.13274900 2.05030800H 3.22899300 1.29725600 1.75743000N 0.37445700 1.67822700 0.44042300H -0.02496600 2.46714400 -0.05649200C -0.77222100 0.58431500 -1.41139400O -0.51336200 -0.06539200 -2.41507900N -1.71957700 1.57041900 -1.42664500H -2.03839400 1.98086600 -0.55980400C -2.48099000 1.85863800 -2.63884900H -3.14692200 1.02877300 -2.90322400H -3.07264300 2.76159100 -2.47128000H -1.79661100 2.02492200 -3.47433900C -0.05036900 0.33399000 -0.02865200C -1.17125500 -0.22568400 0.94915600H -1.89340200 0.59845300 0.99599500C -0.73669900 -0.45958000 2.40347800H 0.03491000 -1.22959400 2.49733800H -0.36419300 0.45924300 2.86350600H -1.60898600 -0.78293000 2.98249600C -1.94936300 -1.44673400 0.39169300H -1.51539800 -2.38812000 0.73763000H -1.95002500 -1.48569400 -0.69956400S -3.69823400 -1.54683600 0.97952800H -4.18312300 -0.54763000 0.20993000C 1.17010700 -0.55704900 -0.31509300C 2.23696700 -0.00468800 -1.04432400C 1.26929900 -1.89742800 0.07175700C 3.36323500 -0.75903900 -1.36415600H 2.18315500 1.03017400 -1.36985000C 2.40021800 -2.66006000 -0.24351700H 0.47409200 -2.37483600 0.62802100C 3.45313600 -2.09531300 -0.96073500H 4.16997900 -0.30389200 -1.93303400H 2.44925100 -3.69782000 0.07641900H 4.33155000 -2.68637500 -1.20641200 SCF energy=-1296.1861331C -2.48999800 2.60334200 0.07349900O -1.41894600 3.20380000 0.12584600C -3.82044800 3.33356300 0.16697200H -3.91477800 4.00254300 -0.69521500H -4.68898900 2.66727700 0.19594600H -3.81827300 3.95644800 1.06666500N -2.56333500 1.24122900 -0.06205700H -3.46856700 0.83855100 -0.26737200C -1.37600000 0.42188100 -0.35381300H -0.78682400 0.93164600 -1.12094000C -1.80804500 -0.90826500 -0.98883500O -1.26500900 -1.34136800 -1.99848800N -2.86518300 -1.55207000 -0.39470500H -3.06963000 -1.31818300 0.56863000C -3.27778400 -2.87365700 -0.85790400H -2.51957000 -3.63437100 -0.63571800H -4.21872400 -3.13918100 -0.36913900H -3.42848400 -2.84559400 -1.93913500C -0.44581200 0.28056600 0.90555900H -0.27946600 1.32208100 1.19689700C 2.01970100 0.59622000 0.14895100C 3.13077700 -0.23594000 -0.15262200C 4.37224700 0.28174100 -0.54538400C 4.48648400 1.66463400 -0.63901000C 3.39346300 2.51203100 -0.34856000C 2.16415900 1.99429900 0.04224400C 0.91366400 -0.25806900 0.52031000C 1.38646400 -1.55416800 0.42355100H 5.21237700 -0.37020500 -0.77185900H 5.43377400 2.10132600 -0.94481400H 3.51711000 3.58799500 -0.43888100H 1.32581600 2.65617100 0.24432200N 2.71944500 -1.53676500 0.02837800H 3.24493100 -2.36844600 -0.19873500S 0.58423900 -3.12485500 0.61278300H 1.01410900 -3.40684300 1.86841900C -1.09876200 -0.40247100 2.11970500H -2.05477700 0.07959500 2.35999300H -1.26405900 -1.47339500 1.97325700H -0.44932100 -0.29020200 2.99500700 SCF energy=-1356.1375271C -2.87978800 2.26319600 0.30948400O -1.93694000 3.05076600 0.24306800C -4.28552400 2.71652800 0.66018400H -4.61430300 3.44392200 -0.08926900H -5.01282700 1.89946000 0.70416600H -4.26208500 3.22795100 1.62760400N -2.72070000 0.92635000 0.06625000H -3.50647100 0.29851600 0.16776900C -1.42976100 0.36840400 -0.32957400H -0.93700500 1.10408900 -0.96946800C -1.66647700 -0.87017400 -1.22034600O -1.48793500 -0.81810000 -2.43228600N -2.17064400 -1.96725400 -0.58451100H -2.02200600 -2.02442900 0.41640300C -2.38985300 -3.21138400 -1.31235400H -1.44343700 -3.69080000 -1.59182200H -2.96540400 -3.89109000 -0.67901900H -2.95168000 -3.00320600 -2.22551600C -0.50725300 0.17187200 0.89531000H -0.51720600 1.11350900 1.45184200C 1.88004800 0.78060700 0.13431200C 3.09402700 0.08423000 -0.10820700C 4.25672500 0.73556300 -0.54046300C 4.18516900 2.11171700 -0.72608900C 2.98698500 2.82353000 -0.49197600C 1.83389400 2.17531200 -0.06663300C 0.90356600 -0.19471200 0.55703300C 1.54375700 -1.41915500 0.56824600H 5.17774200 0.18843700 -0.72483700H 5.06781500 2.65005600 -1.06106700H 2.96768500 3.89788300 -0.65319700H 0.91529900 2.73391700 0.09632800N 2.85960800 -1.24525600 0.16505400H 3.53498400 -1.99528000 0.12854800S 0.99491600 -3.06350400 0.94839900H 0.95475700 -2.93451600 2.29487400F -1.09294000 -0.78597500 1.77165700 SCF energy=-1445.4908574C -2.35273200 2.67845000 -0.04081000O -1.27379100 3.26060300 0.07636100C -3.67726700 3.40407600 0.11876000H -3.73829600 4.19038600 -0.64090500H -4.55112300 2.75129500 0.02390100H -3.69855500 3.89162500 1.09848700N -2.42606200 1.34462600 -0.32339800H -3.33027000 0.89885200 -0.39019000C -1.22951300 0.54312600 -0.57657300H -0.56794900 1.14486900 -1.20326100C -1.57075400 -0.68245100 -1.45115000O -0.97911600 -0.87621200 -2.50759200N -2.59541700 -1.47687400 -1.02107700H -2.82913700 -1.43243600 -0.03572700C -2.93450800 -2.69574400 -1.74617500H -2.15130000 -3.45739000 -1.64472600H -3.87643400 -3.08763100 -1.35336300H -3.05360200 -2.46617200 -2.80727000C -0.38344900 0.27314600 0.71957700H -0.25078300 1.28312900 1.13514100C 2.12124500 0.61312100 0.07989800C 3.22390000 -0.23666700 -0.20707900C 4.48660900 0.26565400 -0.54790900C 4.63111100 1.64766000 -0.60018700C 3.54656800 2.51058500 -0.32324400C 2.29496400 2.00987300 0.01350000C 0.99627500 -0.23323400 0.38747900C 1.44111200 -1.53478600 0.27759900H 5.32055400 -0.39722600 -0.76468900H 5.59669300 2.07225900 -0.86226100H 3.69549700 3.58549100 -0.38053400H 1.46378800 2.68369400 0.20715400N 2.78156700 -1.53469800 -0.07430900H 3.32048600 -2.37330700 -0.23473800S 0.58027200 -3.06904900 0.47121700H 0.72282000 -3.18557500 1.81437400C -1.01912100 -0.47613500 1.88636200O -0.42941000 -0.83724900 2.87918700O -2.37603700 -0.64502900 1.78565500H -2.65715200 -1.06540700 2.62144600 SCF energy= -1594.0120514C -2.46518500 2.53110800 -0.46504800O -1.42824100 3.18681000 -0.37910700C -3.83618000 3.17904300 -0.40340400H -3.88067300 3.97869300 -1.14909700H -4.66119500 2.48017600 -0.57544100H -3.96292200 3.63906000 0.58235300N -2.44677700 1.16887700 -0.60115100H -3.31475200 0.67883000 -0.77106900C -1.19493700 0.43248300 -0.77819500H -0.57776900 0.98349200 -1.49283500C -1.46657500 -0.91391500 -1.48513500O -0.80156900 -1.23982200 -2.46111600N -2.53524200 -1.64662500 -1.04222900H -2.79234100 -1.53487900 -0.06933100C -2.81556700 -2.94926700 -1.64020600H -2.02985500 -3.67788700 -1.40603100H -3.77496900 -3.30877700 -1.25969900H -2.87401800 -2.84291400 -2.72533800C -0.30513600 0.40994300 0.52176200H -0.14417800 1.47484500 0.71900600C 2.20641900 0.65404700 -0.03161400C 3.31536200 -0.20709600 -0.24569200C 4.59052600 0.27567900 -0.56871000C 4.74232300 1.65310600 -0.67793600C 3.65223300 2.52924100 -0.47375700C 2.38942600 2.04619900 -0.15445600C 1.06409900 -0.17537600 0.27184000C 1.51171500 -1.48367300 0.23515200H 5.42743300 -0.39905800 -0.73001700H 5.71689400 2.06374900 -0.92834300H 3.80592000 3.60029900 -0.57348000H 1.55882100 2.73418500 -0.01653500N 2.86311500 -1.49489400 -0.07098300H 3.40451100 -2.34180600 -0.16858100S 0.68314500 -3.03681600 0.43874100H 0.72345600 -3.09065100 1.79206100C -0.99457200 -0.05008400 1.81257000F -0.10769200 -0.22552700 2.81844700F -1.89419700 0.86959300 2.24631800F -1.69228600 -1.22232600 1.70988100 SCF energy= -1782.6247918C -1.09431100 -3.24719500 0.33475300O -0.02631700 -3.50993300 -0.21931200C -2.23381500 -4.24767700 0.40119500H -1.88481900 -5.13958200 0.93193200H -3.12834100 -3.86317600 0.90159900H -2.49714000 -4.55297500 -0.61639000N -1.32139000 -2.03211100 0.91807300H -2.19266500 -1.87364000 1.40537600C -0.26539600 -1.02636700 1.03574600H 0.64318200 -1.54030600 1.35939200C -0.56638200 -0.03817100 2.18261500O 0.28642500 0.20220700 3.02966100N -1.82915400 0.47961500 2.23808900H -2.36497700 0.48432500 1.37967400C -2.17653400 1.46589800 3.25617400H -1.65738500 2.41774400 3.09021600H -3.25667300 1.62945900 3.23006500H -1.89139400 1.08707100 4.24001500C 0.14872300 -0.39961400 -0.34580200H 0.33877500 -1.29149100 -0.96223000C 2.75539100 -0.24786300 -0.43140000C 3.71604500 0.78111400 -0.23328400C 5.09367300 0.54700800 -0.33281500C 5.50104400 -0.74764400 -0.63491400C 4.56273200 -1.78617200 -0.83170000C 3.19698200 -1.55179600 -0.73196400C 1.45505700 0.34549800 -0.25526500C 1.66240000 1.67803200 0.03674400H 5.81653100 1.34419700 -0.17889700H 6.56247900 -0.96563200 -0.71857000H 4.91896200 -2.78677800 -1.06120600H 2.48509800 -2.36198700 -0.87057600N 3.02195400 1.93911200 0.04493900H 3.42090800 2.84012400 0.26561700S 0.49978700 2.95499500 0.42161700H 0.27377200 3.38372700 -0.84486000C -0.86766900 0.35760500 -1.18810100O -0.64337100 0.95851000 -2.19800000O -2.19133500 0.20094400 -0.70568700C -3.24267400 0.69407400 -1.44116400F -4.35850900 0.40400500 -0.74372000F -3.33837300 0.11964700 -2.64543200F -3.18729300 2.02395800 -1.59784300 SCF energy=-1177.4718752C 3.14524500 1.26745100 -0.14196000O 3.95444900 1.69456000 -0.95814600C 3.47266800 1.14600400 1.33696500H 2.89925200 1.87451700 1.92410100H 3.24798600 0.14864800 1.73156600H 4.53539400 1.35534200 1.46638400N 1.88751700 0.87291100 -0.54580900H 1.67827600 1.03878000 -1.52673200C 0.80228200 -1.14692000 0.49645900O 0.09867400 -1.64941200 1.38465500N 1.61345000 -1.86644400 -0.30008400H 2.11896600 -1.36660500 -1.02073000C 1.69876400 -3.31866700 -0.23707900H 0.87694000 -3.79156200 -0.78825700H 2.64988400 -3.63746400 -0.66984300H 1.64767000 -3.63851000 0.80614200C 0.79449400 0.38366500 0.28115700H 0.86735800 0.81756900 1.28374700C -0.52874400 0.90283900 -0.34341600C -1.81478400 0.50623500 0.45214300H -0.45339700 1.99869400 -0.32010800H -1.54546400 0.21056700 1.46592200C -2.59669800 -0.61833200 -0.23915900O -3.15818200 -0.40633900 -1.31710400N -2.64766600 -1.80258100 0.41354900H -1.93439200 -2.01818700 1.10405700H -3.08599000 -2.57521700 -0.07363000S -3.02510800 1.91340300 0.57149800H -2.37098100 2.54288800 1.57384800O -0.53136500 0.46444900 -1.69430800H -1.45084600 0.43919300 -2.02546300 SCF energy=-1157.5957574C -3.22329200 -1.12754500 0.07506900O -4.07498400 -1.61272300 -0.66429300C -3.53791700 -0.70638800 1.50169300H -3.02427400 -1.35496700 2.22274800H -3.22882800 0.32506800 1.70563300H -4.61424600 -0.79865700 1.65406000N -1.93338000 -0.94677300 -0.36466500H -1.72138800 -1.27262600 -1.30674100C -0.73082400 1.13899800 0.36660500O -0.09000700 1.71908500 1.25075200N -1.38708200 1.77990400 -0.62258300H -1.87906400 1.21320500 -1.30164200C -1.35455500 3.22736100 -0.77930800H -0.41131000 3.55736300 -1.23051900H -2.18563800 3.53207500 -1.41954900H -1.45590100 3.70383800 0.19904600C -0.80288400 -0.40040500 0.36401900H -0.86856600 -0.67503600 1.42181400C 0.48541600 -1.08981500 -0.20870800C 1.80323500 -0.62873700 0.48187400H 0.35483800 -2.14182600 0.07029100H 1.65717800 -0.60482800 1.56497300C 2.36343000 0.72401100 0.01248900O 2.44889600 1.00841900 -1.18205100N 2.85541200 1.53336900 0.99232000H 2.42715100 1.49127800 1.90828100H 3.11669100 2.46369900 0.68562400S 3.16935800 -1.85653000 0.14198800H 2.81254200 -2.71757700 1.12042700N 0.47483300 -1.04039100 -1.66913900H 0.96720200 -0.20692500 -1.99276800H 0.98851700 -1.83550200 -2.04267200 SCF energy= -1201.4972248C 2.82262400 1.64171200 -0.04593500O 3.56945700 2.27317200 -0.78409500C 3.01760300 1.59422300 1.45963900H 2.20707100 2.12308900 1.97642300H 3.04516800 0.56740400 1.84201300H 3.96097500 2.09018700 1.69204200N 1.76401700 0.92905700 -0.57540400H 1.62414000 1.07362600 -1.57155300C 0.99533200 -1.34428000 0.19645100O 0.25291700 -2.07452200 0.86109600N 2.06542900 -1.80279100 -0.48322300H 2.60937000 -1.13433100 -1.01291400C 2.41012300 -3.21770800 -0.52339700H 2.41753100 -3.62948600 0.48954000H 1.68530100 -3.78367200 -1.11947800H 3.40249800 -3.32378700 -0.96668300C 0.73901300 0.18188300 0.13883400H 0.70495500 0.52163900 1.17700600C -0.62906000 0.52260400 -0.47880800C -1.87252800 -0.13719500 0.11433000H -0.75905300 1.60817400 -0.47760900H -1.81915000 -1.21622400 -0.03621800C -3.12746500 0.45762700 -0.54758400O -3.21930000 1.65111000 -0.80295300N -4.11476700 -0.44034900 -0.82214800H -4.08399900 -1.38731400 -0.47158100H -5.00733600 -0.08072100 -1.13589600S -2.03645400 0.15641300 1.93913600H -1.26302300 -0.90126600 2.27079300F -0.56693200 0.13081900 -1.84335500 SCF energy=-1290.8455103C 3.27360700 1.17600100 0.17804700O 4.17144500 1.51154100 -0.58856500C 3.49590600 1.03874300 1.67402800H 2.88217000 1.75482700 2.23469300H 3.24548400 0.03401200 2.03346300H 4.54806900 1.24174000 1.87821500N 2.00691800 0.92931700 -0.30644900H 1.93812400 0.98361400 -1.31670800C 0.91816500 -1.16044700 0.65937300O 0.43347800 -1.61273000 1.69964600N 1.53453500 -1.91495600 -0.27495300H 1.76650200 -1.47083900 -1.15362500C 1.49939600 -3.37046900 -0.22442400H 0.51325800 -3.75288500 -0.51426100H 2.26139300 -3.76604300 -0.90064600H 1.71474400 -3.69989400 0.79430300C 0.88226500 0.37210700 0.43011100H 0.92768300 0.77044400 1.44773300C -0.47447300 0.90558100 -0.12982700C -1.69794700 0.41133500 0.69891200H -0.41688000 1.99178400 0.00934900H -1.33204400 0.09750100 1.68074900C -2.31477600 -0.86360200 0.08477700O -1.65455900 -1.54645200 -0.69375500N -3.54802700 -1.21745000 0.51832700H -4.14184500 -0.54909500 0.99082300H -3.97080300 -2.03969100 0.10787100S -2.94631300 1.75579200 1.01343400H -2.69200200 1.88592500 2.33318800C -0.77334000 0.75375300 -1.62146500O -1.81845600 1.10802200 -2.11836100O 0.26057900 0.28932800 -2.37348800H -0.04954300 0.27186400 -3.29958200 SCF energy=-1330.152467C -3.28095200 0.54371300 -1.08883600O -4.17457400 1.33091800 -0.78956500C -3.51566300 -0.62964100 -2.02378000H -2.92250100 -0.52962500 -2.94146800H -3.24666900 -1.58432000 -1.55758200H -4.57374900 -0.64342300 -2.28888200N -2.00875900 0.71937800 -0.59107200H -1.92599600 1.48460300 0.06901000C -0.92392700 -1.43365000 0.22461600O -0.45412400 -2.49887100 -0.18310500N -1.52658500 -1.28743700 1.42422500H -1.73659100 -0.34438400 1.72358800C -1.48235900 -2.33969500 2.43056100H -0.48717400 -2.41000800 2.88608500H -2.22656900 -2.12382000 3.20137400H -1.71794000 -3.29677200 1.96013800C -0.88617800 -0.19895300 -0.71064300H -0.93280800 -0.64822400 -1.70698000C 0.47091800 0.57342200 -0.69998900C 1.69127400 -0.37083700 -0.91809700H 0.41706800 1.22549900 -1.57983700H 1.32373800 -1.29440300 -1.37477900C 2.30921900 -0.81857600 0.42405800O 1.64734000 -0.75076000 1.45669100N 3.54813900 -1.36458800 0.37542100H 4.14323700 -1.22351100 -0.42997300H 3.97193200 -1.64125500 1.25126700S 2.93911600 0.33447600 -2.10645800H 2.70411000 -0.54387200 -3.10496000C 0.77742400 1.54139700 0.44689900O 1.83706400 2.12482400 0.52538700O -0.25067700 1.75983300 1.29713000C 0.01576500 2.68533700 2.37674900H -0.92053400 2.75842700 2.93038000H 0.81437100 2.29092100 3.00878400H 0.30729700 3.65841600 1.97561700 SCF energy=-1194.4802418C 3.24779700 1.07719400 0.12287600O 4.11118100 1.48679700 -0.64325400C 3.54198000 0.72695700 1.57073700H 3.01933400 1.40709800 2.25512400H 3.23316600 -0.29534200 1.81623200H 4.61634000 0.82740100 1.73039300N 1.94497700 0.92742600 -0.31504700H 1.80430500 1.19253500 -1.28671400C 0.76502700 -1.15552400 0.53250000O 0.15772700 -1.66167000 1.47916200N 1.43966800 -1.85518000 -0.40131500H 1.82553100 -1.34338500 -1.18434700C 1.33872700 -3.30548500 -0.49890300H 0.39210600 -3.60107500 -0.96608000H 2.17541400 -3.67953300 -1.09381000H 1.38475300 -3.73615300 0.50358000C 0.82468400 0.38844400 0.43635300H 0.91585100 0.70491800 1.47990100C -0.50994500 1.05310800 -0.06522800C -1.80236400 0.45776900 0.55927300H -0.44222500 2.09053800 0.28269100H -1.56758900 0.13774400 1.57834000C -2.30114000 -0.80096900 -0.18360900O -1.61916300 -1.33122200 -1.05102500N -3.49743500 -1.29384600 0.22407500H -4.09852400 -0.79351400 0.86388600H -3.84763300 -2.12707300 -0.22983200S -3.16528600 1.71888300 0.67025300H -2.72431700 2.30294200 1.80533900C -0.56598900 1.15740900 -1.53369400N -0.52614500 1.34533200 -2.67909300Radicals: SCF energy= -726.4109036 C -2.53809500 1.95571000 -0.07511400O -3.62541700 2.44701100 0.21533400C -1.45807400 2.75673200 -0.78493700H -0.50584500 2.72935800 -0.24433300H -1.27793600 2.36086400 -1.79299100H -1.80009500 3.78913900 -0.87120200N -2.25581400 0.64721300 0.22612900H -3.02746500 0.09366000 0.59320100C -1.43714400 -1.62005000 0.01313700O -2.54991500 -1.97603600 0.38732400N -0.45561400 -2.48867900 -0.33476700H 0.47630800 -2.12762300 -0.49333200C -0.63084300 -3.93092500 -0.20790700H -1.59064100 -4.22212200 -0.64072400H 0.17607900 -4.43002100 -0.74943700H -0.61473800 -4.24877700 0.84174900C -1.06186800 -0.10696100 -0.11540800H -0.80364900 0.05827100 -1.16980300C 0.10931900 0.22465900 0.77067900H -0.13365700 0.34271200 1.82477200C 1.46618100 0.34084400 0.37837400C 2.46272900 0.58258400 1.37445500C 1.91821400 0.22691100 -0.97257600C 3.80484100 0.69477900 1.04418200H 2.14870800 0.67745700 2.41127200C 3.26665100 0.34165400 -1.29103200H 1.20277500 0.06794600 -1.77491600C 4.22186200 0.57320500 -0.29124300H 4.53715000 0.87859400 1.82624900H 3.57943100 0.25621400 -2.32876400H 5.27359300 0.66193200 -0.54819700 SCF energy=-778.1516119C -0.87983800 2.23037400 0.27811900O -0.90668900 3.20613600 1.02088500C -0.43751200 2.33015700 -1.17126100H 0.52690500 1.82693300 -1.31746300H -1.16342200 1.88392700 -1.86060400H -0.31893200 3.38819600 -1.41035100N -1.27703000 0.99324100 0.75112500H -1.41857100 0.98587200 1.75777000C -2.51114700 -0.97873100 -0.23267600O -2.54643200 -2.12770700 -0.66998600N -3.61364900 -0.21755800 -0.04130300H -3.48256200 0.72352000 0.30542100C -4.94855500 -0.70111600 -0.36460000H -5.11791600 -1.67738900 0.09888700H -5.68201600 0.01326200 0.01602700H -5.07889400 -0.81075300 -1.44738000C -1.15187000 -0.32166200 0.10680300H -0.67450500 -0.15074500 -0.86894200C -0.29864400 -1.25806900 0.91722900H -0.70537200 -2.23786300 1.14981100C 1.15777500 -0.99115700 1.10587400C 2.03248300 -1.72309200 0.04484900H 1.48441700 -1.32139600 2.10271200H 1.36807200 0.08378300 1.03923900H 1.95408800 -2.80694900 0.17978500H 1.65462900 -1.50421600 -0.95639300N 3.45345900 -1.37205700 0.10092600H 3.92663300 -1.72332400 0.92610700C 3.92607300 -0.11399800 -0.28127500N 3.26536900 0.42669300 -1.39267100H 3.74500000 1.26669500 -1.70138900H 3.13542100 -0.22681800 -2.15968000N 4.87903300 0.55461600 0.26490700H 5.18912600 0.12904300 1.13998900 SCF energy= -683.9280369C 2.76537700 -0.37424800 0.08829800O 3.76089400 -0.99604700 -0.26694800C 2.85914800 0.87388300 0.95218900H 2.40291500 1.74217100 0.46217100H 2.35141200 0.73233000 1.91466000H 3.91411400 1.08077800 1.13704000N 1.50934900 -0.78854400 -0.28612800H 1.45413900 -1.67090100 -0.79138300C -0.85538200 -1.33507200 -0.10730500O -0.58888200 -2.36045700 -0.72438000N -2.05352800 -1.05960300 0.44269000H -2.17915900 -0.16231200 0.90331300C -3.17891500 -1.97948100 0.32099400H -2.92415400 -2.95581900 0.74456800H -4.02719900 -1.55998600 0.86551200H -3.45603300 -2.12197200 -0.72906800C 0.23758600 -0.21891300 0.10231300H 0.22065500 0.02122300 1.17432900C -0.10549200 1.01412400 -0.67196200H 0.32454900 1.15649000 -1.65820000C -1.01429100 2.00388400 -0.13781500O -1.65883300 1.86998900 0.90482400O -1.10970900 3.11824900 -0.90443400H -1.74793200 3.71609800 -0.47163300 SCF energy=-801.657139C -2.74410400 2.10304900 -0.10652200O -3.80009400 2.67347300 0.15525800C -1.58339900 2.82757400 -0.76969500H -0.65359200 2.71704300 -0.20160400H -1.40384600 2.43334300 -1.77853900H -1.84129100 3.88474400 -0.84876400N -2.57319700 0.77362500 0.18363400H -3.39679900 0.27655400 0.51690200C -1.91857000 -1.54575700 -0.01688500O -3.06986100 -1.82077400 0.30644900N -0.98972700 -2.48419100 -0.32925700H -0.02635100 -2.19234500 -0.43260200C -1.27520900 -3.90969500 -0.21813000H -2.24213200 -4.12473200 -0.67855300H -0.49402000 -4.46516900 -0.74246900H -1.31181100 -4.23518900 0.82888500C -1.42612800 -0.06573700 -0.12098300H -1.12102900 0.08284500 -1.16564200C -0.26307600 0.17599100 0.80429400H -0.52944500 0.29739300 1.85225500C 1.10749100 0.20948800 0.45284700C 2.09222900 0.38228000 1.47425900C 1.60002200 0.08126900 -0.88438400C 3.44697600 0.41989300 1.18824900H 1.76220900 0.48685400 2.50484300C 2.95583500 0.11912300 -1.17058000H 0.90441900 -0.03156400 -1.71124500C 3.89122600 0.28642200 -0.13821200H 4.16798000 0.55342100 1.99322500H 3.31333000 0.02703400 -2.19195300O 5.21349400 0.31180100 -0.48577200H 5.76478100 0.44433900 0.30159700 SCF energy= -668.6137312C -1.40674300 2.19317700 0.08269300O -1.52540200 3.13719000 0.85851100C -1.78706000 2.29707100 -1.38411900H -0.89235000 2.27664800 -2.01885300H -2.43926800 1.47660800 -1.70335200H -2.29940000 3.24853800 -1.53383800N -0.92249200 0.98195800 0.52853100H -0.60177400 1.01090500 1.49188100C -1.76820600 -1.24951000 -0.30155300O -1.67166700 -2.24241000 -1.02153700N -2.84557100 -1.00366900 0.48340400H -2.86160600 -0.14275000 1.01338300C -3.99212800 -1.90097100 0.51679900H -3.66642000 -2.92284300 0.73271300H -4.67686600 -1.56556300 1.29901400H -4.51706300 -1.90744600 -0.44525500C -0.61908800 -0.21596600 -0.24954700H -0.43619900 0.07357800 -1.28895500C 0.66096200 -0.89779100 0.28056400C 1.89787000 -0.07077400 0.13385800H 0.76950800 -1.85287300 -0.24839000H 0.49075400 -1.17270500 1.34202600C 3.25323900 -0.67924500 0.29833000C 4.39529900 0.22837700 -0.17403500H 3.44564000 -0.93895200 1.35623800H 3.29771200 -1.63870600 -0.24403800H 4.23181700 0.49109900 -1.23399200H 4.36808200 1.16600200 0.39550100N 5.69411900 -0.40583900 0.08342100H 5.81176000 -1.23448800 -0.49819000H 6.45829900 0.22650300 -0.14566900H 1.80666800 1.01484500 0.14855100  SCF energy=-703.3702908C 3.14481000 0.58108800 -0.28919000O 4.02877800 0.47234900 -1.13282000C 3.44659400 0.77090200 1.18536100H 2.99102400 1.68968800 1.57562200H 3.06453200 -0.07452900 1.76710900H 4.52954300 0.83681200 1.30006500N 1.81974200 0.56276400 -0.67992300H 1.70710100 0.32597900 -1.66164300C 0.30214400 -1.04798100 0.39055000O 0.99737400 -1.68941500 1.18039000N -0.68662500 -1.60809000 -0.34567000H -1.36398300 -1.02656100 -0.83561800C -1.01271700 -3.02111500 -0.18963100H -1.38568800 -3.23728400 0.81874500H -1.77908600 -3.28023800 -0.92327500H -0.12196500 -3.63240000 -0.35920900C 0.63404900 0.44983500 0.16092600H 0.89027600 0.83577000 1.14994700C -0.48943300 1.34444800 -0.44327700C -1.72905200 1.44426900 0.37296300H -0.74105400 0.99959900 -1.45241800H -0.04291600 2.34360500 -0.54425400H -1.70114600 1.98147500 1.31968200C -2.98249400 0.84090200 -0.07186600O -3.03312900 0.07929400 -1.05364200N -4.10160700 1.12810500 0.66270200H -4.10555900 1.82460900 1.39390000H -4.98925100 0.76210700 0.34514900 SCF energy=-668.6124889C 2.02640400 1.97163900 -0.10162800O 2.42679300 2.82331200 -0.88989600C 2.45612400 1.94936400 1.35492700H 1.62060900 2.22993000 2.00846900H 2.80710100 0.96060900 1.67030400H 3.25792600 2.67809800 1.48234200N 1.16117100 0.98478700 -0.52261700H 0.84636700 1.11238200 -1.47984900C 1.27887400 -1.39903400 0.30686600O 0.90662500 -2.29975900 1.05786800N 2.33915800 -1.51956500 -0.52926400H 2.61327700 -0.71012100 -1.06976800C 3.14343900 -2.73260200 -0.58019600H 2.49783600 -3.60506700 -0.71515900H 3.83564800 -2.65962000 -1.42217000H 3.71378800 -2.87118100 0.34568500C 0.51236100 -0.05648200 0.27008500H 0.45941300 0.27425100 1.31266400C -0.92864600 -0.29995200 -0.22529300C -1.88503700 0.89029700 0.04151300H -1.30317700 -1.19602000 0.27868300H -0.90782000 -0.52618000 -1.30146800C -3.27731100 0.63826900 -0.44571300H -1.89191900 1.08110100 1.12638300H -3.56242500 0.92589600 -1.45563000H -1.47796900 1.79367300 -0.43255000C -4.34597000 0.08601200 0.43976100H -3.88365200 -0.54033600 1.22730200H -4.85417600 0.90761000 0.97815400N -5.38043400 -0.60659700 -0.34027800H -5.00177600 -1.44983500 -0.76805500H -6.15709500 -0.88905500 0.25405100 SCF energy=-801.6579214C 2.53161100 -2.06740000 -0.15533800O 3.58132600 -2.63595000 0.13417600C 1.39411400 -2.79215700 -0.85666900H 0.48522800 -2.79570300 -0.24500400H 1.14391400 -2.31524200 -1.81278400H 1.70976600 -3.81955000 -1.04427400N 2.34405700 -0.74338600 0.15296400H 3.16114400 -0.24970000 0.50715400C 1.69928800 1.58248400 0.01017700O 2.85905500 1.84402300 0.31357400N 0.75313800 2.53162600 -0.19185400H -0.21002700 2.23914900 -0.29273900C 1.03914400 3.94755500 0.00554800H 1.95350000 4.21726900 -0.52870000H 0.20428200 4.53058300 -0.39004800H 1.17802700 4.18542700 1.06702500C 1.22436600 0.10804900 -0.21445700H 1.02737200 0.02388300 -1.29280700C -0.01908700 -0.19653900 0.57564500H 0.14100600 -0.40492200 1.62839200C -1.34202200 -0.20520000 0.08000900C -2.43421800 -0.47832300 0.97368400C -1.69484200 0.04325300 -1.28313900C -3.75087600 -0.49405300 0.52873100C -3.01233700 0.02497200 -1.72082300H -0.90721200 0.24059600 -2.00441800C -4.04978100 -0.24288300 -0.81681100H -4.55302200 -0.70453300 1.23453100H -3.23579100 0.21430200 -2.76699200H -5.08298800 -0.25957100 -1.15115800O -2.10350700 -0.71937600 2.27850000H -2.90271700 -0.90779900 2.79470500 SCF energy=-840.9628502C 2.61383800 -2.17420500 -0.22321200O 3.56315500 -2.85692100 0.15405100C 1.56305200 -2.71909300 -1.17724800H 0.56435900 -2.69892100 -0.72732000H 1.51834200 -2.12897900 -2.10141900H 1.82954600 -3.74741900 -1.42607700N 2.46416900 -0.88126400 0.20923200H 3.23707500 -0.49891200 0.75058600C 1.99687000 1.49033400 0.24205600O 3.09378500 1.62099300 0.77658200N 1.17617700 2.53393400 -0.03217600H 0.23105100 2.33808700 -0.33571100C 1.51850900 3.89650400 0.35714300H 2.53624800 4.12759900 0.03319800H 0.82067800 4.58347100 -0.12721100H 1.46481700 4.03070500 1.44430500C 1.46519000 0.08941800 -0.20699500H 1.41439700 0.12668400 -1.30413700C 0.10667900 -0.18930100 0.37879100H 0.10904000 -0.51411600 1.41362300C -1.13389100 -0.03550800 -0.27670300C -2.35956600 -0.30472100 0.43881000C -1.27270500 0.37837700 -1.63660700C -3.59836000 -0.16282800 -0.17969800C -2.51417500 0.51684300 -2.24459700H -0.37975100 0.57811300 -2.22193700C -3.68055800 0.24828400 -1.51936400H -4.51173300 -0.36912900 0.36660100H -2.57504300 0.82868300 -3.28358900H -4.65572300 0.35279000 -1.98651500O -2.19880600 -0.69805200 1.73184300C -3.34921100 -1.00669500 2.51180500H -3.91346600 -1.83838300 2.07173800H -2.96939200 -1.30043100 3.49140400H -4.00197600 -0.13112400 2.61818000 SCF energy= -1186.0171882C 3.37650900 -1.38811600 -0.39997700O 4.23257500 -2.02593200 0.20465100C 3.55223600 -0.95044700 -1.84194700H 2.76567100 -1.36700200 -2.48361600H 3.51942600 0.14094300 -1.92686800H 4.52050200 -1.31588200 -2.18720100N 2.18749700 -1.07385200 0.22768400H 2.18251000 -1.32973100 1.21049300C 1.49876600 1.29717900 0.23313000O 2.22712100 2.00636500 -0.45634200N 1.02181800 1.67407200 1.44541700H 0.31599700 1.09390100 1.88096800C 1.30891000 2.98526000 2.01363500H 0.77033700 3.77983200 1.48317700H 1.01021000 2.98537400 3.06453000H 2.38004800 3.18919800 1.94181400C 1.14588900 -0.15698000 -0.22746200H 1.19985300 -0.11039100 -1.31905100C -0.20561300 -0.65431600 0.20352700H -0.22443800 -1.48041200 0.90646200C -1.43279300 -0.15471700 -0.29167700C -2.69912800 -0.66688500 0.13876100C -1.48580900 0.89477200 -1.26294200C -3.90097700 -0.18372300 -0.35948500C -2.68632200 1.37739200 -1.75999900H -0.55619500 1.32614700 -1.62185600C -3.90259800 0.84159700 -1.31315100H -4.83438200 -0.60793500 -0.00346100H -2.68005000 2.17412700 -2.49858400H -4.84647800 1.21468300 -1.69981900Cl -2.76942400 -1.95199700 1.33884400 SCF energy=-915.0306184C 3.43834700 -1.41274800 -0.69549900O 4.21871600 -2.24369800 -0.24168000C 3.71105600 -0.65463100 -1.98107900H 2.92561100 -0.83579300 -2.72550700H 3.76389000 0.42382800 -1.79723900H 4.66399600 -1.00494400 -2.38041900N 2.24650100 -1.16668900 -0.04353300H 2.17742500 -1.65260100 0.84551700C 1.72695600 1.18244000 0.51470400O 2.51856700 1.98594800 0.02867800N 1.24020900 1.28488700 1.77649800H 0.48989500 0.66303800 2.05058500C 1.59326900 2.39537700 2.65213500H 1.12582600 3.33084900 2.32193300H 1.25929900 2.16256000 3.66594800H 2.67728500 2.53370200 2.65107600C 1.29276100 -0.08802500 -0.29033600H 1.39581300 0.20918000 -1.33735200C -0.10607200 -0.56677200 -0.01110800H -0.19672200 -1.51250200 0.50535300C -1.27918400 0.12001900 -0.40811300C -2.62156600 -0.34784300 -0.14067500C -1.16543600 1.33337100 -1.15997000C -3.71819700 0.35607300 -0.65371200C -2.27091800 2.01773200 -1.63616400H -0.17920500 1.73132700 -1.37558700C -3.56248700 1.52807700 -1.39279000H -4.70942600 -0.03518300 -0.45047700H -2.13047400 2.93355100 -2.20432300H -4.43459000 2.05437300 -1.76933100C -2.99713700 -1.54813800 0.65970800O -4.10580500 -2.05191500 0.65449800O -2.01512200 -2.05320300 1.45926700H -2.41477700 -2.81541600 1.92035400 SCF energy= -1063.554117C -3.55815200 1.49731300 -0.61749700O -4.28005500 2.35400700 -0.11840200C -3.91165000 0.78397800 -1.90889700H -3.14283700 0.94213200 -2.67553200H -4.01474200 -0.29440500 -1.74676100H -4.85788600 1.19136500 -2.26797300N -2.35764800 1.17831200 -0.01295800H -2.23665400 1.63881300 0.88423900C -1.94487300 -1.20666400 0.48857500O -2.77308800 -1.97461900 0.00606100N -1.44509000 -1.33981200 1.74214000H -0.66921000 -0.74966900 2.01477000C -1.83478800 -2.43994000 2.61571800H -1.41563400 -3.39292200 2.27132400H -1.47428000 -2.23011000 3.62536100H -2.92387600 -2.52873200 2.63142400C -1.47467700 0.05456900 -0.31136000H -1.63073500 -0.21995600 -1.35839000C -0.04086200 0.44689900 -0.08330600H 0.12081100 1.39337200 0.41900800C 1.07244700 -0.31877400 -0.51264200C 2.43312800 0.07190900 -0.25253800C 0.88802500 -1.53452900 -1.23796200C 3.49649600 -0.70221700 -0.70414000C 1.96079900 -2.29451000 -1.68154700H -0.11905300 -1.87697700 -1.45336900C 3.27348200 -1.88466000 -1.42090600H 4.51245800 -0.38504200 -0.49689200H 1.77483500 -3.21161200 -2.23398700H 4.11671200 -2.47461000 -1.76707300C 2.73515400 1.32756900 0.52545300F 4.06053600 1.52662000 0.70311400F 2.17976900 1.30441600 1.77382800F 2.25272000 2.44541900 -0.08198700 SCF energy=-818.6730145C 3.29927200 -1.35057100 -0.46388700O 4.17573000 -1.98517900 0.11248400C 3.44634400 -0.86946000 -1.89517000H 2.66228600 -1.28819100 -2.53848600H 3.38715300 0.22271500 -1.95279400H 4.41859200 -1.20224400 -2.26152200N 2.11029400 -1.08036600 0.18717400H 2.12195300 -1.36857900 1.16103800C 1.38074200 1.28514400 0.25031800O 2.01236500 2.04938500 -0.47449500N 0.99574600 1.60215400 1.51088200H 0.37693600 0.96885800 2.00065300C 1.29671400 2.89854300 2.10711300H 0.72632700 3.70133200 1.62554700H 1.04391600 2.86174400 3.16908900H 2.36157900 3.11903800 1.99615500C 1.04994000 -0.16842800 -0.23013600H 1.08134000 -0.09919100 -1.32101200C -0.28923300 -0.68538100 0.21397000H -0.29135900 -1.50477700 0.92865200C -1.52820300 -0.20780200 -0.26873000C -2.77207300 -0.76383500 0.20259900C -1.62191300 0.83315400 -1.24041200C -3.99942300 -0.30488300 -0.28763700C -2.84773100 1.27590500 -1.71390700H -0.71367400 1.29234200 -1.61860400C -4.04470900 0.71063400 -1.24489700H -4.91674700 -0.74868900 0.08717800H -2.87851700 2.06934500 -2.45567100H -5.00197700 1.05935500 -1.62023800C -2.76473500 -1.79579300 1.19415700N -2.75068600 -2.62751300 2.00991900 SCF energy= -957.5139118C 3.31305400 2.02688800 0.97904000O 3.70450100 3.15726700 0.70344700C 3.96210200 1.18125900 2.05891200H 3.24110100 0.91078800 2.84049300H 4.37149300 0.25660000 1.63842700H 4.76565200 1.76832700 2.50610100N 2.22375100 1.49947200 0.31724900H 1.89556800 2.09385400 -0.43792900C 2.50242200 -0.71028100 -0.73664600O 3.59477700 -1.20788100 -0.47487300N 1.93159200 -0.77169600 -1.96607000H 0.96673600 -0.47850600 -2.05085500C 2.55269800 -1.49145200 -3.07012200H 2.49165700 -2.57760100 -2.92901800H 2.04496100 -1.21875900 -3.99854200H 3.60696700 -1.21292800 -3.13956700C 1.73313400 0.12322400 0.34019100H 2.04230600 -0.32163000 1.29132100C 0.23221200 0.11038600 0.22566900H -0.24585800 1.06728600 0.04356000C -0.58188400 -1.02738700 0.45393600C -2.02060400 -0.94603200 0.38683900C -0.00761100 -2.28670000 0.81060200C -2.78325700 -2.07028600 0.71009600C -0.79368900 -3.38876900 1.11097200H 1.07282100 -2.38473300 0.86360800C -2.19087000 -3.28677200 1.07003700H -3.86664400 -1.99670900 0.65787900H -0.32134500 -4.32924100 1.38253200H -2.81331600 -4.14566100 1.30532000C -2.72817200 0.30745200 -0.00575600C -3.60906300 0.93415100 0.89167500C -2.57325700 0.86552700 -1.28681700C -4.30661600 2.08763200 0.52369900H -3.73566300 0.51933300 1.88858400C -3.27299800 2.01545000 -1.65800400H -1.91628100 0.37969100 -2.00430100C -4.14035700 2.63293500 -0.75186200H -4.97730800 2.56118300 1.23621400H -3.14512100 2.42593700 -2.65656600H -4.68282200 3.52990400 -1.03888400  SCF energy= -613.2670183C 2.30525400 -0.56363600 -0.02288100O 2.74838400 0.53679400 0.31275200C 3.23254000 -1.69457500 -0.44475200H 3.87144900 -1.96025400 0.40438100H 2.70612800 -2.59098500 -0.78765100H 3.88587600 -1.33394800 -1.24555000N 0.97680500 -0.85444200 -0.05245100H 0.65945900 -1.79625200 -0.26510000C -1.40790200 -0.73162200 0.05121000O -1.40445800 -1.95065100 -0.13140100N -2.54090800 0.00698500 0.03676100H -2.43796100 1.01416300 0.05104800C -3.84583400 -0.57917500 -0.23576000H -3.98277300 -1.47437000 0.37622600H -4.61819300 0.15151500 0.01604300H -3.94796200 -0.86522600 -1.28973400C -0.09575900 0.05030900 0.40133500C -0.04992400 1.38510700 -0.32651900C 0.28406500 2.67024700 0.36859700H -0.15573300 2.75296500 1.36857900H 1.37567700 2.76895600 0.49045200H -0.05848000 3.52926800 -0.22259300C 0.06723200 1.35439200 -1.82242000H -0.37021600 0.45079700 -2.26300200H -0.41810600 2.22844600 -2.27726100H 1.12526800 1.38431600 -2.13549800C -0.04678900 0.17439900 1.94359200H -0.87110400 0.78673700 2.32355300H -0.12425900 -0.82106000 2.39236600H 0.90095400 0.62531800 2.24836000 SCF energy= -629.3179036C 2.39449700 -0.47139200 0.23092100O 2.70140300 0.48069300 0.95250200C 3.45013400 -1.40577100 -0.33906200H 4.03468000 -1.82421300 0.48665600H 3.03568400 -2.22488100 -0.93536700H 4.13577100 -0.82152500 -0.96191000N 1.10337900 -0.76712900 -0.08863900H 0.88371400 -1.50257600 -0.75322800C -1.29570700 -0.72977400 -0.18150900O -1.22759400 -1.49792000 -1.14434200N -2.43459300 -0.44522200 0.48601800H -2.32939800 0.11193200 1.32704800C -3.71336100 -1.05071200 0.14857500H -3.80626300 -2.06274100 0.56299200H -4.51793300 -0.42660600 0.54590800H -3.80834600 -1.11645200 -0.93790700C -0.04079900 0.06528800 0.31320800C -0.03792500 1.41290800 -0.39978500C 0.30868500 1.47473800 -1.85478200H 0.95856800 0.65487700 -2.17140600H -0.59484400 1.43485100 -2.48991700H 0.81264900 2.42219200 -2.08930000C -0.74954500 2.59531300 0.18283200H -0.84459300 2.54136300 1.26961700H -0.21803700 3.52225200 -0.07377100H -1.76901300 2.70172200 -0.23325700N -0.13764500 0.24834900 1.76144500H -0.04944800 -0.66132300 2.21494600H 0.67248400 0.79336700 2.05945600 SCF energy= -673.215434C 2.31785900 -0.56233700 0.00453900O 2.74748600 0.56998200 0.18414200C 3.23488800 -1.75403800 -0.21546900H 3.52589500 -2.16254400 0.76009600H 2.76568900 -2.55519500 -0.79606200H 4.14038400 -1.41331900 -0.72254100N 0.97489400 -0.86662400 -0.00089900H 0.67009400 -1.82971300 -0.12408800C -1.41047300 -0.73823000 -0.03589100O -1.39576100 -1.93245800 -0.33039600N -2.53343500 0.00047200 0.04781300H -2.44280100 0.96707300 0.33306300C -3.85827300 -0.58370500 -0.11331900H -4.10318000 -1.24727200 0.72413800H -4.59256100 0.22330300 -0.16163400H -3.89868800 -1.16608800 -1.03778700C -0.08547700 0.03189200 0.32351700C 0.00673900 1.40052100 -0.29327100C 0.27877800 2.61995700 0.52881400H -0.09844200 2.53166600 1.55143300H 1.36412400 2.79878700 0.60051600H -0.16827800 3.50724600 0.06047200C 0.15419300 1.46811000 -1.78270100H -0.28816900 0.60423200 -2.29302400H -0.31481500 2.37683800 -2.18197700H 1.21859900 1.50560400 -2.07003600F -0.16791800 0.16991400 1.74463900  SCF energy=-687.2894121C -2.37493400 -0.52016800 -0.30297600O -2.69459300 0.64919400 -0.52549000C -3.40773500 -1.62651200 -0.17854600H -4.02622900 -1.63592200 -1.08149600H -2.96998100 -2.61882800 -0.03238800H -4.06572700 -1.39867100 0.66681900N -1.07289600 -0.89829900 -0.16569800H -0.81183600 -1.85120000 0.07239200C 1.32687300 -0.82816500 0.02125400O 1.22902000 -2.01105100 0.34991300N 2.49990000 -0.18728100 -0.13833800H 2.47449400 0.74480000 -0.53853100C 3.77566900 -0.87754700 -0.00018000H 3.94359300 -1.58212100 -0.82369700H 4.57407100 -0.13233300 0.00466700H 3.79594900 -1.43573600 0.93934200C 0.03399500 0.05862000 -0.17297700C -0.03947000 1.05993800 0.97905200C -0.20938000 2.53267300 0.76181600H 0.50455300 2.95011200 0.04294500H -1.21777300 2.76044000 0.37768200H -0.08750500 3.06861900 1.70994200C -0.27668900 0.49675800 2.34844900H 0.06417000 -0.53955600 2.44888000H 0.23535500 1.10037800 3.10964100H -1.34983400 0.51165400 2.60963600C 0.10067000 0.72358600 -1.55877100O 0.97313600 1.50297500 -1.88604700H -0.68682100 0.41337400 -2.26730100C 2.35750500 0.56719200 0.21545100O 2.74521600 -0.59178500 0.15607200C 3.30516600 1.74899500 0.30044100H 3.54726200 2.08174600 -0.71643700H 2.87916300 2.59790900 0.84565200H 4.22992100 1.42641500 0.78340600N 1.02119400 0.90592000 0.19088400H 0.73901200 1.88330700 0.20893400C -1.37125300 0.84151200 0.22433400O -1.29941000 2.05127800 0.42810900N -2.51798200 0.14081700 0.19990100H -2.46925200 -0.81711600 -0.12671200C -3.81736300 0.79476800 0.30011100H -4.06914000 1.32991200 -0.62342300H -4.57584400 0.03377100 0.49582000H -3.80190400 1.51234200 1.12347400C -0.05106100 -0.00323900 -0.01279300C -0.00852200 -1.26890400 0.80798500C 0.45933900 -2.60266400 0.31092300H 0.70321900 -2.62095000 -0.75167100H 1.36365500 -2.90537000 0.85742400H -0.30499700 -3.37393100 0.49496900C -0.10358400 -1.08334900 2.29425600H -0.67269300 -0.19392400 2.58592700H -0.57426700 -1.95826300 2.76193800H 0.90094800 -0.98936200 2.74075800N -0.12499400 -0.38382500 -1.56826800O -1.00746700 -1.17907700 -1.89049400O 0.66616400 0.14299300 -2.32892600  SCF energy=-778.4899087C 2.35750500 0.56719200 0.21545100O 2.74521600 -0.59178500 0.15607200C 3.30516600 1.74899500 0.30044100H 3.54726200 2.08174600 -0.71643700H 2.87916300 2.59790900 0.84565200H 4.22992100 1.42641500 0.78340600N 1.02119400 0.90592000 0.19088400H 0.73901200 1.88330700 0.20893400C -1.37125300 0.84151200 0.22433400O -1.29941000 2.05127800 0.42810900N -2.51798200 0.14081700 0.19990100H -2.46925200 -0.81711600 -0.12671200C -3.81736300 0.79476800 0.30011100H -4.06914000 1.32991200 -0.62342300H -4.57584400 0.03377100 0.49582000H -3.80190400 1.51234200 1.12347400C -0.05106100 -0.00323900 -0.01279300C -0.00852200 -1.26890400 0.80798500C 0.45933900 -2.60266400 0.31092300H 0.70321900 -2.62095000 -0.75167100H 1.36365500 -2.90537000 0.85742400H -0.30499700 -3.37393100 0.49496900C -0.10358400 -1.08334900 2.29425600H -0.67269300 -0.19392400 2.58592700H -0.57426700 -1.95826300 2.76193800H 0.90094800 -0.98936200 2.74075800N -0.12499400 -0.38382500 -1.56826800O -1.00746700 -1.17907700 -1.89049400O 0.66616400 0.14299300 -2.32892600  SCF energy=-805.042303C 2.05054300 -1.61744400 -0.33812700O 1.92413700 -2.11174600 0.78110700C 3.01170500 -2.20856300 -1.36116800H 2.73570900 -3.25297800 -1.53991500H 3.02635100 -1.67352800 -2.31602200H 4.02083900 -2.20622200 -0.93606600N 1.36348400 -0.51761300 -0.75662400H 1.47631000 -0.17412400 -1.70675000C 0.20092000 1.55575400 -0.82836200O 0.43519100 1.56032700 -2.03710600N -0.25671300 2.64199100 -0.17057700H -0.29938800 2.59773300 0.83908200C -0.51402600 3.90336000 -0.85193400H -1.17356200 3.73765900 -1.70837100H -0.99881500 4.58614300 -0.15031900H 0.41488200 4.35755000 -1.21626300C 0.37203400 0.23637500 0.02813100C 0.90482000 0.55720700 1.42083700C 0.46816300 -0.14295300 2.67239900H -0.43899000 -0.73567500 2.54701700H 1.25884400 -0.83029800 3.00870600H 0.30086100 0.57772200 3.48888900C 2.22108300 1.27919200 1.50080700H 2.43169400 1.89916800 0.62254000H 2.26451200 1.92110300 2.39208300H 3.05116100 0.55910700 1.59830000C -1.01834100 -0.44564600 0.01091500C -1.26423900 -1.57578000 -0.77658800C -2.08990700 0.09720900 0.73845100C -2.53486400 -2.15699300 -0.82616100H -0.45874100 -2.01072300 -1.35692900C -3.36039100 -0.47784400 0.69083200H -1.93708900 0.97510700 1.35955700C -3.58969300 -1.61168000 -0.09370800H -2.69517900 -3.03857100 -1.44172600H -4.17022000 -0.03926900 1.26870800H -4.57804500 -2.06236800 -0.13205900 SCF energy=-613.2345286C 2.14505400 -1.13583100 -0.22210300O 2.52181600 -2.08892300 -0.90392200C 3.12150300 -0.41312200 0.68802500H 3.14608000 0.66465900 0.50636700H 2.87008500 -0.57279800 1.74118000H 4.11015700 -0.83208400 0.49386600N 0.81834700 -0.76143300 -0.29884500H 0.33218800 -1.39220600 -0.92876300C -1.43044400 -0.38809300 0.48176800O -1.91544600 -0.58507300 1.58950000N -2.05766400 -0.81299000 -0.65628800H -1.73794100 -0.48473100 -1.55667200C -3.35555700 -1.47689500 -0.59577100H -4.14494000 -0.79026000 -0.26712200H -3.59807300 -1.86082800 -1.58958800H -3.31059000 -2.30836500 0.11172800C -0.03376300 0.29636900 0.28933400C -0.17596900 1.51950800 -0.72480300H -0.50027200 1.07171900 -1.67874700C 1.16005000 2.22214300 -1.01558200H 1.54290700 2.75009500 -0.13484500H 1.92077400 1.51497300 -1.35925800H 1.01780300 2.96662500 -1.80667900C -1.22054500 2.49403700 -0.28279800H -2.27662400 2.24142600 -0.31001300H -0.94111300 3.43561200 0.18101100C 0.42738800 0.77058700 1.67071800H 0.55644700 -0.07591500 2.34831100H 1.35634700 1.33878100 1.62010900H -0.34527700 1.41400600 2.09770700 SCF energy=-629.2943093C 2.08209500 0.94396400 -0.20947300O 2.84847400 1.62952900 -0.88105500C 2.58516600 0.00271600 0.86706900H 2.00849400 0.07636600 1.79316100H 2.52045500 -1.03677500 0.52472700H 3.63210100 0.24197800 1.06078000N 0.72328200 0.99914800 -0.46306700H 0.50402600 1.69598700 -1.16671700C -0.27851900 -1.13782100 0.33053600O -0.43818300 -1.75727700 1.38043500N 0.00578200 -1.74577300 -0.84595000H 0.26284300 -1.16720500 -1.63387800C 0.14241000 -3.19241800 -0.94745800H -0.74091100 -3.68083600 -0.52688700H 0.23644900 -3.46152100 -2.00197300H 1.02369200 -3.55197700 -0.40276700C -0.41609700 0.41954500 0.27067100C -1.71018000 0.76973600 -0.56072600H -1.52991800 0.46178700 -1.60161800C -1.99912900 2.29379100 -0.56019200H -2.17221300 2.64327600 0.46160100H -1.18522300 2.88634000 -0.99933400H -2.90004100 2.49514700 -1.14934700C -2.89643000 0.02444300 -0.03829300H -3.72894900 -0.20039100 -0.69769900H -3.01814000 -0.13005600 1.02853700N -0.56869900 0.90458100 1.63478800H -0.36342500 0.16948000 2.30770300H -0.01001300 1.73095600 1.81547400 SCF energy= -673.1845837 C 2.14302300 -1.13025900 -0.22354200O 2.56677800 -2.10288200 -0.83888100C 3.01701800 -0.36469600 0.74679700H 2.90774800 0.71777900 0.66818200H 2.75185800 -0.64533600 1.77193000H 4.05207600 -0.65266900 0.55447300N 0.81148800 -0.77240200 -0.40412500H 0.31707400 -1.47631800 -0.94279400C -1.43327300 -0.39106900 0.45258900O -1.84040700 -0.57995700 1.58578700N -2.10845700 -0.79331100 -0.66643600H -1.84597000 -0.40209500 -1.56135200C -3.43859800 -1.38702600 -0.55735200H -4.19179000 -0.64422000 -0.26757400H -3.70743900 -1.82328500 -1.52228600H -3.41990800 -2.17204500 0.20128700C -0.03194800 0.25606200 0.18658900C -0.15118100 1.55434300 -0.66063900H -0.50008200 1.23949000 -1.65697700C 1.20954900 2.25539100 -0.88958600H 1.63367000 2.60719500 0.05527700H 1.92356900 1.58609900 -1.38180400H 1.06375400 3.12590900 -1.53763400C -1.15673500 2.49045200 -0.06357400H -1.62203900 3.25101200 -0.68310000H -1.30401600 2.53921900 1.01042200F 0.47357500 0.60808800 1.42921500  SCF energy=-687.2552579C 2.05505200 -1.37649300 -0.11458000O 2.41355100 -2.48409900 -0.50335300C 3.04834500 -0.42014400 0.51807600H 2.76154700 0.63092300 0.49570400H 3.19929300 -0.71771700 1.56269400H 4.00343300 -0.54406200 0.00174700N 0.71613800 -1.04028400 -0.21846600H 0.18138400 -1.82674200 -0.57430800C -1.49521100 -0.31817200 0.44607400O -1.95966600 -0.16099600 1.57048700N -2.16714800 -0.97344200 -0.54111600H -1.83092600 -0.90891400 -1.49277300C -3.52646300 -1.46488700 -0.32930400H -4.24870400 -0.64171700 -0.27471800H -3.79030300 -2.12801700 -1.15631300H -3.56873600 -2.02179500 0.60913600C -0.05639700 0.17340700 0.09191700C -0.11759900 1.19804400 -1.11663700H -0.47497800 0.58881900 -1.96325600C 1.25505400 1.75394700 -1.53102800H 1.67756500 2.39594500 -0.75270100H 1.96561500 0.95424400 -1.76236900H 1.13578200 2.35891800 -2.43641400C -1.10811500 2.29384800 -0.87670700H -2.17621300 2.10863300 -0.94723900H -0.78280800 3.25095100 -0.48482200C 0.43538600 0.79999400 1.41695500O 0.61451900 1.98235800 1.58844700H 0.61758100 0.06125600 2.21946200 SCF energy=-778.4534187C 2.00540000 -1.38762100 -0.28294400O 2.32243400 -2.54929600 -0.49679100C 3.05232100 -0.35158400 0.06469400H 3.82999800 -0.37481600 -0.70459300H 2.69223100 0.66807300 0.18212000H 3.51085100 -0.66724100 1.00759700N 0.64326200 -1.07181200 -0.32913900H 0.10676200 -1.93234800 -0.27935800C -1.56765200 -0.28230400 0.32848200O -2.12159700 0.13519600 1.33100000N -2.15885800 -1.13206600 -0.55634400H -1.71299600 -1.32405500 -1.44372200C -3.54531200 -1.55626400 -0.37243600H -4.24274800 -0.72746000 -0.53913700H -3.75808700 -2.36101100 -1.07928600H -3.68287700 -1.92330000 0.64711900C -0.10091300 0.12943200 -0.04273800C -0.16860100 1.16657900 -1.23969800H -0.55652400 0.52544000 -2.04752800C 1.17909800 1.71548400 -1.73416700H 1.64944800 2.36507700 -0.99047300H 1.87511400 0.91937400 -2.01163500H 0.99518200 2.31579300 -2.63160400C -1.15665000 2.26912500 -1.01623600H -2.22239500 2.06695800 -0.97631700H -0.81668600 3.26225900 -0.74713700N 0.43675900 0.78529000 1.27816900O 0.47301000 2.00740500 1.33280700O 0.78845800 0.01923200 2.16241100 SCF energy= -1099.6669134C -0.04128700 2.23972100 -1.24032100O -0.18689100 2.78835200 -2.32713400C 1.00482200 2.73624700 -0.26285300H 0.86221900 3.81282200 -0.13001200H 1.00789200 2.25811100 0.71564100H 1.98564500 2.59278900 -0.72778900N -0.84012300 1.14375200 -0.94772700H -1.34771400 0.85891400 -1.77903600C -1.53062000 -1.12352800 -0.34539700O -0.99293100 -2.20205600 -0.13668900N -2.69221400 -0.99651700 -1.04475800H -3.19144200 -0.11692200 -1.02529400C -3.40189700 -2.17405300 -1.53999600H -3.86843400 -2.73628400 -0.72263500H -4.17016600 -1.84644400 -2.24385200H -2.69754700 -2.83228700 -2.05285800C -0.90865400 0.21340800 0.18272900C -1.85055200 0.74202100 1.35903300H -2.78787000 0.97106900 0.82960600C -1.38572100 2.05286900 2.01370900H -0.45304300 1.92048500 2.57014300H -1.25722600 2.85388200 1.28028000H -2.15303400 2.37921700 2.72398800C -2.13736000 -0.30897000 2.38472800H -2.82502300 -1.12287400 2.17566300H -1.55730300 -0.35518100 3.29954600C 0.48319500 -0.19443200 0.70855100O 0.80985500 -0.28937800 1.85629500O 1.33617500 -0.43417000 -0.35978300C 2.61202500 -0.89749700 -0.12448700F 3.35057600 -0.00503900 0.55928400F 2.62390700 -2.05792900 0.53717600F 3.17952200 -1.07976900 -1.32331400 SCF energy= -933.2097899C -2.71400300 2.17037600 -0.03307900O -1.75167300 2.88760900 -0.30407500C -4.08515700 2.74860200 0.27205800H -4.42761800 3.31349200 -0.60116500H -4.83639800 1.99191100 0.52062700H -3.99565500 3.45268500 1.10537800N -2.61814900 0.80665900 -0.00110100H -3.40418100 0.25956900 0.32243300C -1.35962700 0.11720300 -0.27190500H -0.83788700 0.69462100 -1.03711800C -1.66218300 -1.25430100 -0.91516200O -1.54428800 -1.42294600 -2.12519900N -2.13859200 -2.21302500 -0.07196300H -1.98303600 -2.06489200 0.92079200C -2.42047700 -3.55712000 -0.55647200H -1.50301400 -4.08546900 -0.84588300H -2.92627900 -4.11658800 0.23470200H -3.07042700 -3.50425300 -1.43355300C -0.44311600 0.10352900 0.97977500H -0.35536500 1.15319100 1.28796800C 2.07192800 0.31840800 0.20667800C 3.18611500 -0.56269400 0.17686000C 4.44751800 -0.16099700 -0.26708400C 4.59182700 1.16894200 -0.65991700C 3.50495900 2.06612100 -0.61869500C 2.24403800 1.65594300 -0.19377000C 0.92623800 -0.43442000 0.69873000C 1.39978500 -1.70888000 0.85255400H 5.28690800 -0.85107300 -0.29622400H 5.56210600 1.52000900 -1.00090100H 3.65253400 3.09486500 -0.93596400H 1.40806400 2.35092400 -0.18815100N 2.74534200 -1.80981200 0.63798300H 3.22908400 -2.68095400 0.47049100O -1.11937500 -0.63239500 2.01887900H -0.52340900 -0.69719800 2.78185600 SCF energy= -972.5154566C -2.64352500 2.22240800 -0.21733700O -1.65804300 2.92998200 -0.42344000C -4.01843200 2.81639000 0.03803200H -4.32754500 3.37480900 -0.85192500H -4.78466700 2.06896000 0.26856200H -3.94971700 3.52865800 0.86607600N -2.57135600 0.85744500 -0.21807800H -3.38417800 0.31506100 0.04021300C -1.31953100 0.15039100 -0.47455200H -0.76974100 0.72983000 -1.21857900C -1.63643500 -1.20312400 -1.14865200O -1.51852500 -1.34679400 -2.36191700N -2.12612400 -2.17399900 -0.32740900H -1.97811600 -2.04575900 0.66922800C -2.41616200 -3.50633300 -0.83866000H -1.50076200 -4.03869700 -1.12720800H -2.93597300 -4.07469700 -0.06302200H -3.05589000 -3.43138500 -1.72159700C -0.42724200 0.09455400 0.79508400H -0.33063000 1.13653600 1.13168100C 2.10544500 0.31598800 0.07848000C 3.20770200 -0.57827900 0.00616000C 4.48008400 -0.16881800 -0.39704600C 4.64942800 1.18132500 -0.70188900C 3.57513400 2.09056300 -0.61705200C 2.30265400 1.67328600 -0.23546900C 0.94287300 -0.44870200 0.50707000C 1.39316100 -1.73792900 0.57765900H 5.30942400 -0.86873800 -0.46077100H 5.62922400 1.53843400 -1.00767400H 3.74175600 3.13487900 -0.86710700H 1.47622300 2.37875400 -0.19965000N 2.74139600 -1.84521400 0.37924100H 3.21271800 -2.71047300 0.15508700O -1.12230200 -0.64902300 1.80357200C -0.64120600 -0.43669300 3.12573400H -0.72948700 0.62319500 3.40451900H -1.26809100 -1.03873000 3.78817900H 0.40530400 -0.75172500 3.22661900 SCF energy=-1317.5783034C 3.04721600 1.92717500 0.70598500O 2.29604800 2.49205400 1.49694200C 4.35208600 2.55156000 0.24430100H 4.97687100 2.74403100 1.12243800H 4.91255300 1.92970700 -0.46123200H 4.13501500 3.51672700 -0.22425100N 2.76115300 0.68883300 0.19335700H 3.36183400 0.29407100 -0.51726500C 1.54545600 -0.02823400 0.55073100H 1.34946000 0.17875800 1.60651900C 1.80496000 -1.54989600 0.47555900O 1.83615300 -2.23028400 1.49768600N 2.07363400 -2.05729400 -0.76008500H 1.79201700 -1.50783600 -1.56538600C 2.29508900 -3.48619400 -0.94767400H 1.37439500 -4.06303500 -0.79354400H 2.66063300 -3.65299000 -1.96383000H 3.04152000 -3.83717700 -0.23146500C 0.29731400 0.50757500 -0.18916000H 0.23909500 1.57771300 0.00990800C -2.31779400 0.36655200 0.01442000C -3.22510600 -0.60194100 0.52102100C -4.60769800 -0.40448700 0.53700400C -5.08439000 0.80440300 0.03402300C -4.20364000 1.78095800 -0.47412200C -2.82688100 1.57389400 -0.49253700C -0.96794800 -0.16754800 0.15488000C -1.16066900 -1.40953200 0.69987700H -5.28526200 -1.15905000 0.92817800H -6.15390500 0.99628900 0.03380300H -4.60902900 2.71182700 -0.86145000H -2.16072100 2.33113000 -0.89647500N -2.46380200 -1.69397800 0.94774800H -2.81405300 -2.54683400 1.35865200Cl 0.57865400 0.50846200 -2.06909500 SCF energy=-971.322344C -2.46488300 2.30898900 0.05764000O -1.37379500 2.88297800 0.06615500C -3.77369600 3.06829000 0.17338000H -3.85608400 3.75742700 -0.67374500H -4.65416200 2.41865200 0.19292200H -3.75345400 3.67242700 1.08600800N -2.56391600 0.95142500 -0.03824400H -3.45793100 0.50106700 -0.21697700C -1.40882200 0.11730100 -0.30434500H -0.77127400 0.61491400 -1.04415400C -1.94263900 -1.20363600 -0.90380400O -3.15565100 -1.39538700 -1.02955700N -1.00926000 -2.10111000 -1.28680600H -0.04686700 -1.93577400 -1.01094400C -1.37874300 -3.41784300 -1.79274600H -2.12540600 -3.31242500 -2.58356900H -0.48513700 -3.89565100 -2.20049200H -1.79921000 -4.04974300 -1.00143200C -0.51072300 -0.07585700 0.98533100H -0.52256500 0.92207500 1.44993400C 1.94298000 0.39574100 0.12781100C 3.16117100 -0.33856600 0.13907100C 4.35982900 0.18749400 -0.35060300C 4.33119300 1.49171000 -0.84063300C 3.13973300 2.24643100 -0.84026100C 1.94417500 1.71565800 -0.36253100C 0.90817600 -0.45667300 0.69981100C 1.54854400 -1.63206000 0.98601900H 5.28062300 -0.39042000 -0.33961400H 5.24663700 1.93704500 -1.22125100H 3.15612700 3.26488300 -1.21930900H 1.03340000 2.30909000 -0.35793300N 2.88428800 -1.58527500 0.70111400H 3.52436500 -2.36305400 0.76383200C -1.19592600 -1.00962400 1.96375800O -0.67783700 -1.97934500 2.47905800H -2.25079400 -0.75589600 2.19165800 SCF energy=-1062.5186325C -2.66977400 2.21355900 -0.74566400O -2.19050600 2.34085700 -1.86735200C -3.61053600 3.24514800 -0.14854600H -4.43076200 3.42371500 -0.85066000H -4.02343700 2.95312500 0.82220100H -3.06796700 4.18972700 -0.03408200N -2.40839600 1.11803600 0.04834000H -2.70278600 1.11663400 1.01843200C -1.40578400 0.12563600 -0.31041600H -1.11452700 0.36496700 -1.33965400C -1.96531200 -1.31302700 -0.32369600O -1.23009800 -2.28624000 -0.14964100N -3.28419100 -1.42863200 -0.59395000H -3.83249600 -0.58134100 -0.64823700C -3.94180500 -2.72639900 -0.66851000H -3.99824000 -3.19962800 0.31843000H -4.95137600 -2.58417200 -1.06052200H -3.38427600 -3.38954000 -1.33557700C -0.11186700 0.24256000 0.53160400H 0.05016100 1.30940500 0.71918400C 2.45103800 0.23632100 -0.04707500C 3.31778000 -0.68080200 -0.70253800C 4.68038500 -0.43253800 -0.88445600C 5.18567700 0.76595700 -0.38486800C 4.34877200 1.68855600 0.27537500C 2.99072600 1.43568900 0.44859900C 1.11714000 -0.34345400 -0.05454200C 1.25753900 -1.53711600 -0.70713700H 5.32400800 -1.14697400 -1.39156200H 6.24210800 0.99069500 -0.50395800H 4.77372200 2.61284300 0.65778000H 2.36394500 2.15782000 0.96656000N 2.54069800 -1.77488400 -1.08768200H 2.86030700 -2.57994400 -1.60578700N -0.38207300 -0.28440900 1.98219600O 0.54934800 -0.73318000 2.62213400O -1.53306000 -0.14251800 2.41440300 SCF energy=-1089.0682849C -1.35140000 3.02865100 0.24033300O -0.25928400 3.26784500 0.75466000C -2.52218400 3.99002500 0.36049200H -2.27421200 4.91221800 -0.17645400H -3.46122600 3.59164700 -0.03764300H -2.66050700 4.25084700 1.41401100N -1.58381200 1.88641200 -0.47329600H -2.48573100 1.75673500 -0.91148600C -0.51765400 0.93252000 -0.78674100H 0.38092700 1.50706300 -1.02042800C -0.86883400 0.19203200 -2.08923100O -0.13285000 0.24054100 -3.06789800N -2.08384300 -0.44234300 -2.11502000H -2.48890400 -0.71065000 -1.22524100C -2.48895700 -1.21154900 -3.28700100H -1.87128900 -2.10844700 -3.42195100H -3.53523500 -1.50455700 -3.16905600H -2.38536800 -0.59175600 -4.18042900C -0.13496200 0.02807900 0.45658700H 0.09570600 0.77530300 1.22320600C 2.48248200 -0.11725500 0.33473400C 3.44043900 -1.12408000 0.04131500C 4.81550300 -0.88764800 0.08723000C 5.23202000 0.38746800 0.46886400C 4.29928100 1.39561000 0.78670300C 2.92809200 1.15986400 0.72163000C 1.15427400 -0.70007400 0.17679800C 1.40419600 -1.96310700 -0.27886500H 5.53478800 -1.66709200 -0.15164800H 6.29539500 0.60466500 0.52669100H 4.65806000 2.37895400 1.07918700H 2.21877400 1.95185200 0.94933400N 2.73367300 -2.28757400 -0.28535300H 3.12241100 -3.05001800 -0.82248000C -1.27741900 -0.81345200 1.01380000C -2.11978700 -0.25150200 1.98850500C -1.53942700 -2.13209300 0.60456300C -3.18877400 -0.97155200 2.52871200H -1.92222200 0.75793400 2.34061900C -2.60615100 -2.85799500 1.14376500H -0.89872700 -2.60410900 -0.13600600C -3.43849300 -2.27956400 2.10590700H -3.81767700 -0.51339200 3.28809100H -2.77939200 -3.88004800 0.81552900H -4.26409200 -2.84597800 2.52912600 SCF energy=-817.9105391C -3.27352700 0.47950900 -0.12044800O -4.14433600 0.87108500 0.65043000C -3.59879200 -0.16084200 -1.45787300H -3.21040100 0.44058400 -2.29003600H -3.16489600 -1.16347700 -1.53449400H -4.68454300 -0.22029400 -1.54600100N -1.94341400 0.63788100 0.20798000H -1.78368700 0.99977200 1.14285400C -0.43016600 -1.32426900 -0.00732700O -0.89832500 -2.28821900 -0.61876900N 0.33150600 -1.44135700 1.10131100H 0.78867600 -0.61101100 1.46464900C 0.71058500 -2.74560000 1.62653000H 1.36630500 -3.28231300 0.93053100H 1.23610400 -2.59790500 2.57224100H -0.18094900 -3.35623500 1.79534100C -0.77921500 0.11091100 -0.48404300H -1.02597400 -0.00132200 -1.54147300C 0.37641500 1.15623200 -0.38627100C 1.57976000 0.72926400 -1.17635000H -0.02091100 2.07033600 -0.86480500H 1.45954500 0.79451000 -2.25692600C 2.82958500 0.16577700 -0.66319200O 3.09412300 0.04057400 0.53761800N 3.74479800 -0.19001600 -1.63395000H 3.47179600 -0.31151300 -2.59951300H 4.55992400 -0.70176200 -1.32064000O 0.57945700 1.41719900 0.99040700C 1.35122700 2.58012100 1.28544500H 0.92708500 3.45964900 0.77978600H 1.29025400 2.72028700 2.36663100H 2.39886000 2.44341300 0.99815200 SCF energy= -837.3503187C -3.00648900 0.82939400 -0.08312500O -4.19354600 0.62914800 0.16425500C -2.51570500 2.18456600 -0.57513500H -1.68186600 2.56733400 0.02464700H -2.17413400 2.12199100 -1.61627600H -3.34976100 2.88602700 -0.52195900N -2.07377200 -0.16122400 0.07282900H -2.44348700 -1.08693700 0.28067300C -0.27958900 -1.55784900 -0.73659300O -0.94306300 -2.53370600 -0.37570800N 0.76858700 -1.62764900 -1.57711800H 1.30879700 -0.77597900 -1.72012600C 1.29998600 -2.90568100 -2.02345500H 0.48748000 -3.53996800 -2.38768400H 2.00902000 -2.72455900 -2.83497600H 1.81032700 -3.43661200 -1.20946900C -0.66127100 -0.12838300 -0.26647900H -0.51082200 0.55095400 -1.10719400C 0.22915900 0.38375800 0.94637800C 1.08307100 1.57556400 0.62656500H -0.50213000 0.76659500 1.68247000H 1.21758400 2.29703000 1.43003900C 1.80971000 1.83601200 -0.61231200O 1.88443600 1.03651100 -1.56094600N 2.46053100 3.04277700 -0.67270300H 2.33396000 3.76457600 0.02199700H 2.92805300 3.28711300 -1.53564400N 0.99242800 -0.71889200 1.59495700C 2.23370300 -0.32767700 2.25723200H 2.90598700 0.17028600 1.55095300H 2.08384900 0.33807900 3.12963800H 2.73215300 -1.23500800 2.61377800C 0.14579400 -1.49377400 2.50483800H 0.70904600 -2.36427800 2.85672700H -0.17236200 -0.90262100 3.38530400H -0.73895600 -1.86030200 1.98305100 SCF energy=-1162.9674725C 3.22777800 0.62389600 0.14138600O 4.16903100 0.79629100 -0.62356000C 3.42002700 0.44518800 1.63578300H 2.84054500 1.17607900 2.21409700H 3.11254000 -0.56107700 1.93871200H 4.47970200 0.58335600 1.85566400N 1.93542500 0.62721700 -0.35312300H 1.90491600 0.62809400 -1.36879600C 0.52827900 -1.34280000 0.14561600O 1.47509000 -2.06076300 0.47183600N -0.63522300 -1.82358000 -0.32544500H -1.42375400 -1.21397600 -0.53960000C -0.83993100 -3.26111600 -0.45930000H -0.71040600 -3.76609000 0.50400300H -1.85495200 -3.42750700 -0.82570800H -0.12086800 -3.68922500 -1.16540700C 0.72852100 0.19555000 0.32465300H 0.89675200 0.31639300 1.40020400C -0.41492700 1.21266600 -0.00907700C -1.62060700 1.17421600 0.86740800H 0.05721800 2.18582000 0.15452700H -1.50799000 1.69983500 1.81489900C -2.91229300 0.53534200 0.59953100O -3.07941800 -0.33335500 -0.26611400N -3.93942300 0.92801700 1.41951100H -3.87979200 1.75682100 1.99421300H -4.86162100 0.56491200 1.21485000Cl -0.80449800 1.22999700 -1.79479700 SCF energy= -816.7032375C 3.22245200 0.59322700 0.04725200O 4.10748500 0.77780000 -0.77877900C 3.51444900 0.40275200 1.52322700H 2.95514000 1.11029300 2.14767200H 3.25307300 -0.61468100 1.83370600H 4.58258900 0.56446600 1.67524800N 1.89813700 0.58436400 -0.36205800H 1.82234300 0.58582100 -1.37527400C 0.50869400 -1.39176800 0.10019900O 1.36091100 -2.18008800 0.51086300N -0.56243000 -1.77862600 -0.62780800H -1.33662400 -1.13965300 -0.80383800C -0.78564200 -3.19236600 -0.91367700H -0.95986900 -3.76300600 0.00609700H -1.65812200 -3.27653500 -1.56502700H 0.08835900 -3.61696500 -1.41528300C 0.74112800 0.11903800 0.39123900H 1.01592200 0.13774300 1.44755400C -0.42740200 1.16245000 0.22937500C -1.62141100 0.89321200 1.09010800H 0.01338400 2.09723600 0.60363500H -1.54953900 1.11963700 2.15233600C -2.86628500 0.35985900 0.55202400O -2.92730300 -0.09941400 -0.60400800N -3.95190600 0.34916600 1.38126400H -3.96547600 0.86430400 2.25024500H -4.83960500 0.05959200 0.99130900C -0.79426900 1.48127200 -1.23337100O -1.22293600 2.56666800 -1.55440300H -0.60370800 0.70164100 -1.99579600 SCF energy=-907.9105178C 3.21561500 0.40195700 0.35235600O 4.15025500 0.78761800 -0.33878700C 3.42619400 -0.35868100 1.65025800H 3.03814600 0.20187900 2.50998300H 2.93010400 -1.33604300 1.63655000H 4.49921200 -0.50361100 1.78238200N 1.91497600 0.67347200 -0.03205500H 1.83858700 1.11048600 -0.94461300C 0.23340200 -1.26317400 0.10190800O -0.30904200 -1.99226700 0.93491900N 0.47715900 -1.61549900 -1.17490700H 0.74615600 -0.87962600 -1.81559900C -0.04524400 -2.85631100 -1.73555000H -1.12404500 -2.78242400 -1.91613300H 0.47197000 -3.06155300 -2.67568800H 0.13847500 -3.67369000 -1.03518400C 0.70905600 0.14028900 0.56855500H 0.91029700 -0.01806500 1.63122100C -0.44665700 1.18840600 0.58001000C -1.68063100 0.72549600 1.27776700H -0.05808000 2.07911900 1.08477700H -1.76148100 0.93205900 2.34098400C -2.70201700 -0.06079600 0.58328500O -2.61092300 -0.30945500 -0.62246000N -3.77736400 -0.45821300 1.33877300H -3.71849500 -0.48334500 2.34771200H -4.40665000 -1.12341700 0.90701600N -0.79312300 1.74336300 -0.81983700O -1.65106500 2.61050900 -0.84611400O -0.14348000 1.35775300 -1.79115400 SCF energy=-1229.1215059C 3.34768900 -0.52205300 -0.87480200O 3.86124000 -1.63201800 -0.93368400C 4.12612300 0.74655500 -1.17886500H 3.71686000 1.26973900 -2.05179600H 4.11901700 1.44365100 -0.33269500H 5.15621800 0.46030100 -1.39508800N 2.01887900 -0.39596500 -0.50984200H 1.55425800 -1.28804900 -0.36885700C 0.89984500 1.24413000 1.06080900O 0.24093500 2.26831600 1.25176900N 1.42771700 0.50189500 2.05409200H 1.92152600 -0.34461200 1.80558300C 1.17472900 0.80185300 3.45807900H 0.12951300 0.60338000 3.72031900H 1.82716700 0.17685900 4.07137400H 1.38739700 1.85547300 3.65773500C 1.22636300 0.81288500 -0.38972100H 1.82605700 1.63937300 -0.78060500C -0.05230400 0.77689700 -1.30915800C -0.84462600 2.04341100 -1.22100100H 0.34385200 0.70505300 -2.33150700H -0.37563100 2.95031400 -1.59206200C -2.15451800 2.09788100 -0.58824300O -2.73359300 1.07118000 -0.21274200N -2.73416300 3.34282300 -0.48341900H -2.14211800 4.16296600 -0.46347000H -3.56125200 3.38704500 0.09943100C -0.91520300 -0.48466900 -1.18238900O -1.50867300 -1.00212700 -2.08212400O -0.77768600 -1.06051300 0.08954300C -1.47603100 -2.20517700 0.40193700F -2.79065400 -2.07752900 0.24497800F -1.05159100 -3.25770800 -0.32207400F -1.21776300 -2.46384700 1.69641300  |

1. \* Corresponding author. Tel.: +86 21 67791216; fax: +86 21 67791220.

E-mail address: wrzheng@sues.edu.cn (W.R. Zheng). [↑](#footnote-ref-1)