**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 |

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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |

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**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=-1125.2582643  C -0.89008300 2.43691200 -0.30295400  O -0.51368800 3.47735700 0.22475000  C -1.71904500 2.42444200 -1.57456300  H -1.10693500 2.09716500 -2.42466400  H -2.58079100 1.75170400 -1.50993400  H -2.06298000 3.44179100 -1.76687700  N -0.57354700 1.21491600 0.26313900  H 0.13075800 1.29324600 0.99081300  C -2.21312500 -0.64801400 -0.03465300  O -2.69404400 -1.56963600 -0.69873400  N -2.86356100 -0.07970600 1.00655400  H -2.43478100 0.72371600 1.44765500  C -4.19904700 -0.50524200 1.40390200  H -4.21397300 -1.58373700 1.58560300  H -4.47417100 0.02100600 2.32051400  H -4.93430800 -0.28100500 0.62279100  C -0.79266500 -0.10414400 -0.33015400  H -0.70332300 -0.04859100 -1.41905500  C 0.28287800 -1.11472400 0.19576800  H 0.00709500 -1.39256500 1.21882000  S 0.34373500 -2.67302200 -0.81520300  H -0.99613100 -2.81423300 -0.94184000  C 1.68627300 -0.53312200 0.22812200  C 2.36391100 -0.42062000 1.44967000  C 2.32922000 -0.09991300 -0.94229500  C 3.65200400 0.12218300 1.50757400  H 1.88567500 -0.76914600 2.36315800  C 3.61216400 0.44426100 -0.88644000  H 1.82875400 -0.20265100 -1.90161000  C 4.27768000 0.55884400 0.33923700  H 4.16234100 0.19914400 2.46408300  H 4.09577800 0.77703600 -1.80117800  H 5.27784000 0.98206400 0.37969400  SCF energy=-1012.1042809  C 1.15114300 -2.42334700 -0.03870200  O 1.58760100 -3.27320600 0.73124200  C 1.16092500 -2.60867200 -1.54430400  H 0.15435000 -2.52584300 -1.97131500  H 1.79567800 -1.85593300 -2.02500300  H 1.55551700 -3.60360700 -1.75531400  N 0.60522500 -1.25983900 0.46992500  H 0.76969200 -1.16655100 1.46783400  C 1.47981000 0.90820600 -0.21738400  O 2.30221000 0.87400700 -1.12824500  N 1.66020300 1.64732800 0.91415900  H 0.85043300 1.83353000 1.49012800  C 2.77898500 2.57735600 1.02684100  H 2.64512100 3.45216700 0.37800600  H 2.86186500 2.90340100 2.06668800  H 3.69922100 2.06844800 0.73364100  C 0.25389700 -0.04401200 -0.25542300  H 0.14969800 -0.30752800 -1.30946300  C -1.10975100 0.54542300 0.20780500  H -1.03998400 0.87507600 1.25338600  C -2.28013000 -0.48903700 0.10630400  H -2.02826700 -1.17977500 -0.71096800  C -2.40264800 -1.30454900 1.40991400  H -3.20337200 -2.04748000 1.31575300  H -1.48479200 -1.84041000 1.65969300  H -2.66319100 -0.64808300 2.25193900  C -3.65387700 0.12186600 -0.21931200  H -3.96828700 0.84110700 0.54960800  H -3.66763100 0.62531600 -1.18942700  H -4.40782500 -0.67355600 -0.24328800  S -1.30554700 2.09056400 -0.82260500  H -2.37608300 2.58244600 -0.16720900  SCF energy=-969.3962918  C -1.90458300 -1.56099200 -0.02714400  O -2.54971900 -2.36285900 0.64000500  C -2.21588000 -1.30015000 -1.49127500  H -2.36823100 -0.23485800 -1.69305100  H -1.40124400 -1.65738000 -2.13443000  H -3.12287500 -1.85211300 -1.74261800  N -0.86735800 -0.85986100 0.55133400  H -0.59690800 -1.19993800 1.47150200  C 1.51976400 -0.52238900 0.27163600  O 1.74044800 -0.97431300 1.39366900  N 2.45178100 -0.45767300 -0.71130200  H 2.24127700 0.12229200 -1.51334700  C 3.84982300 -0.78445100 -0.45502200  H 3.89975600 -1.70674900 0.12693300  H 4.35895600 -0.93145600 -1.41066000  H 4.35492100 0.00984000 0.10918800  C 0.10686200 -0.00201000 -0.08884300  H -0.04412200 -0.00470800 -1.17066900  C -0.01268900 1.45960300 0.40372100  H 0.14505800 1.48684700 1.48828100  S -1.66480500 2.23547800 0.04831500  H -2.30913700 1.72627900 1.11960100  O 0.97708300 2.19354500 -0.28640200  H 0.98619200 3.10839300 0.03938500  SCF energy=-1200.504245  C -1.07023700 2.45078500 -0.33662100  O -0.59664900 3.47033300 0.15235500  C -1.97555300 2.47856800 -1.55471600  H -1.44360800 2.09350800 -2.43405000  H -2.87720000 1.87100600 -1.42353700  H -2.25759000 3.51489100 -1.74642200  N -0.79729900 1.21667500 0.22676300  H -0.03637300 1.25576100 0.89863500  C -2.56861900 -0.53114000 0.00235600  O -3.13963600 -1.40979700 -0.64812600  N -3.13412500 0.07225300 1.07369200  H -2.63269500 0.84274100 1.49669000  C -4.48146700 -0.25576800 1.51949600  H -4.57875600 -1.33604900 1.65875500  H -4.66834200 0.25101000 2.46884900  H -5.23121500 0.06237800 0.78584700  C -1.12434900 -0.09083000 -0.34221300  H -1.06264900 -0.05777800 -1.43422400  C -0.10776700 -1.16788300 0.17225700  H -0.38428300 -1.41986100 1.20183100  S -0.17888900 -2.73296100 -0.82849200  H -1.52742900 -2.78115600 -0.93092400  C 1.33114000 -0.68653200 0.17796400  C 2.04182200 -0.61416600 1.38157700  C 1.99097500 -0.30413100 -1.00337500  C 3.36556400 -0.16555700 1.41917000  H 1.56354800 -0.92084300 2.30968100  C 3.30578300 0.14670000 -0.98164100  H 1.47237800 -0.37255600 -1.95596500  C 3.99827800 0.21859800 0.23456600  H 3.89826200 -0.12097200 2.36731100  H 3.81305700 0.44342200 -1.89457600  O 5.29029900 0.66777000 0.19169600  H 5.66955800 0.68108300 1.08446300  SCF energy=-1008.7138098  C -2.30825300 1.25211000 -0.11989900  O -3.17020600 1.43283700 -0.97313100  C -2.52515900 1.66314500 1.32990100  H -2.26611200 0.87094800 2.04085200  H -1.91993400 2.54533000 1.57594000  H -3.57782200 1.92323600 1.45103000  N -1.10654400 0.66809800 -0.44639300  H -0.93981300 0.55641400 -1.44446700  C 1.31779500 0.79908700 -0.50161300  O 1.22486800 0.87548000 -1.72478200  N 2.48739100 0.94285700 0.16894500  H 2.49787900 0.67913900 1.14754200  C 3.75183600 1.11415200 -0.53486000  H 3.63856100 1.87764300 -1.30793700  H 4.51044400 1.43629300 0.18256800  H 4.08110600 0.18495800 -1.01722300  C 0.07015900 0.54867600 0.38673000  H 0.05709400 1.31406400 1.17044600  C 0.12910200 -0.81501100 1.13072700  H -0.84061100 -0.95487200 1.62574400  C 0.42592100 -2.04423700 0.25931900  H 1.31274400 -1.87084600 -0.35763300  H 0.63288700 -2.88686300 0.92775700  S -1.01759400 -2.50468600 -0.80316400  H -0.57171000 -3.75137600 -1.07407000  O 1.15589500 -0.65965300 2.12833800  H 1.14799500 -1.42261500 2.72697900  SCF energy=-1102.2199986  C 3.29528600 0.94364800 -0.24321900  O 4.20287400 1.00786000 -1.06608800  C 3.52651300 1.15304100 1.24200100  H 2.94706500 2.00546000 1.61836100  H 3.23629300 0.26701600 1.81682200  H 4.58832600 1.35492200 1.39018300  N 2.00169600 0.70501900 -0.66546000  H 1.94788500 0.48568800 -1.65584200  C 0.80259800 -1.15038700 0.42401700  O 1.28092600 -1.59085300 1.47114800  N 0.33611000 -1.95260400 -0.56643600  H -0.27950600 -1.55834400 -1.26874900  C 0.32680700 -3.40278800 -0.41364500  H -0.37326200 -3.72417700 0.36764300  H 0.03510700 -3.84991500 -1.36645200  H 1.32578800 -3.75054900 -0.13933500  C 0.83569400 0.37566800 0.15162800  H 0.98614500 0.82191500 1.13696400  C -0.41182200 1.02354400 -0.48614200  C -1.71492700 0.82712600 0.30800100  H -0.57402000 0.66948400 -1.51074200  H -0.18589800 2.09314400 -0.55834100  H -1.50322900 0.81699600 1.38314200  C -2.47008700 -0.44756700 -0.09580300  O -2.41585300 -0.92059200 -1.22703000  N -3.24245000 -0.99470300 0.88504600  H -3.17201800 -0.70831200 1.85151900  H -3.74560800 -1.84854500 0.67906800  S -2.79320400 2.30322000 -0.04186400  H -3.89324000 1.86467800 0.60827000  SCF energy= -1256.8824138  C -3.22830700 1.75753300 0.39668500  O -2.36796200 2.63671800 0.29722600  C -4.67220100 2.08655000 0.73392100  H -5.05983300 2.78133400 -0.01824100  H -5.32193300 1.20669700 0.77781600  H -4.70142700 2.60008700 1.70056200  N -2.93990300 0.43972100 0.22007900  H -3.66301700 -0.27277700 0.22337500  C -1.61976200 -0.01520200 -0.17315500  H -1.21406200 0.69883900 -0.89827100  C -1.79996400 -1.38990000 -0.83748500  O -2.82976800 -2.04992600 -0.67861700  N -0.76406200 -1.81779800 -1.59829800  H 0.08559400 -1.26831000 -1.60326000  C -0.75032400 -3.14342000 -2.20403400  H -1.68983000 -3.31515100 -2.73542500  H 0.07960000 -3.19492200 -2.91260200  H -0.63286800 -3.92986400 -1.44884400  C -0.65361100 -0.07509600 1.05511800  H -0.92343300 -0.93421700 1.67892100  H -0.85410900 0.83189400 1.63610100  C 1.56442700 0.96873500 0.12682700  C 2.90647200 0.52146300 -0.01922000  C 3.91435100 1.34105400 -0.54536000  C 3.55490700 2.63044100 -0.92366000  C 2.22873600 3.09769500 -0.77888300  C 1.22985700 2.28376300 -0.25767700  C 0.80360600 -0.11653400 0.70274200  C 1.69494600 -1.15618600 0.89060400  H 4.93704500 0.98727900 -0.65024800  H 4.31140400 3.29377900 -1.33496300  H 1.98890200 4.11441200 -1.07831300  H 0.21340500 2.65266100 -0.14103500  N 2.95743100 -0.77456500 0.44887800  H 3.76909100 -1.37478200 0.46843700  S 1.41450400 -2.79135500 1.50669300  H 1.81217900 -2.58649300 2.78690000  SCF energy=-1200.5065099  C 0.12291700 2.25133000 0.72341900  O -0.34778700 3.25494300 0.19707100  C 0.17091700 2.08127100 2.23154900  H -0.51442500 1.28883300 2.55415900  H 1.17462300 1.82594300 2.59038500  H -0.14374800 3.02268900 2.68436600  N 0.66513100 1.25174800 -0.06182100  H 0.44817500 1.37590400 -1.04847500  C 2.49905800 -0.41432800 -0.09650300  O 2.93165100 -1.56669900 -0.17081700  N 3.27754900 0.66305400 -0.35018200  H 2.84111200 1.57507000 -0.33183400  C 4.67460300 0.52321300 -0.73688700  H 4.76695800 0.02360400 -1.70767100  H 5.12027800 1.51849800 -0.79838800  H 5.21579200 -0.07234500 0.00441200  C 1.03946000 -0.10151300 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-0.12499300  O 2.89172200 -1.56638500 -0.20767800  N 3.23171700 0.66606600 -0.40638000  H 2.78507900 1.57378200 -0.39246900  C 4.61625500 0.53257000 -0.83695300  H 4.68131100 0.06275500 -1.82508000  H 5.06573100 1.52713300 -0.87982100  H 5.17310900 -0.08772300 -0.12866500  C 1.01917900 -0.10239600 0.35164100  H 1.04082000 -0.14823000 1.44388100  C 0.02435500 -1.22056100 -0.13741000  H 0.34494600 -1.53425500 -1.13377000  S 0.15095800 -2.75083800 0.90913100  H 1.47135700 -2.90815600 0.67118800  C -1.41665100 -0.73526300 -0.19073700  C -1.89127400 -0.07797200 -1.34972400  C -2.28984700 -0.88032600 0.89509900  C -3.20295600 0.41521200 -1.38151800  C -3.59559200 -0.38667700 0.86078500  H -1.94001000 -1.38974700 1.78870600  C -4.04995800 0.26825300 -0.28452000  H -3.55641000 0.92513100 -2.27562200  H -4.24731400 -0.51489400 1.72038700  H -5.06241900 0.66060300 -0.33083200  N -1.01583600 0.17756400 -2.43829600  H -0.49258800 -0.63485100 -2.75504000  H -1.49629100 0.58865600 -3.23319300  SCF 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-3.67369000 -1.03518400  C 0.70905600 0.14028900 0.56855500  H 0.91029700 -0.01806500 1.63122100  C -0.44665700 1.18840600 0.58001000  C -1.68063100 0.72549600 1.27776700  H -0.05808000 2.07911900 1.08477700  H -1.76148100 0.93205900 2.34098400  C -2.70201700 -0.06079600 0.58328500  O -2.61092300 -0.30945500 -0.62246000  N -3.77736400 -0.45821300 1.33877300  H -3.71849500 -0.48334500 2.34771200  H -4.40665000 -1.12341700 0.90701600  N -0.79312300 1.74336300 -0.81983700  O -1.65106500 2.61050900 -0.84611400  O -0.14348000 1.35775300 -1.79115400  SCF energy=-1229.1215059  C 3.34768900 -0.52205300 -0.87480200  O 3.86124000 -1.63201800 -0.93368400  C 4.12612300 0.74655500 -1.17886500  H 3.71686000 1.26973900 -2.05179600  H 4.11901700 1.44365100 -0.33269500  H 5.15621800 0.46030100 -1.39508800  N 2.01887900 -0.39596500 -0.50984200  H 1.55425800 -1.28804900 -0.36885700  C 0.89984500 1.24413000 1.06080900  O 0.24093500 2.26831600 1.25176900  N 1.42771700 0.50189500 2.05409200  H 1.92152600 -0.34461200 1.80558300  C 1.17472900 0.80185300 3.45807900  H 0.12951300 0.60338000 3.72031900  H 1.82716700 0.17685900 4.07137400  H 1.38739700 1.85547300 3.65773500  C 1.22636300 0.81288500 -0.38972100  H 1.82605700 1.63937300 -0.78060500  C -0.05230400 0.77689700 -1.30915800  C -0.84462600 2.04341100 -1.22100100  H 0.34385200 0.70505300 -2.33150700  H -0.37563100 2.95031400 -1.59206200  C -2.15451800 2.09788100 -0.58824300  O -2.73359300 1.07118000 -0.21274200  N -2.73416300 3.34282300 -0.48341900  H -2.14211800 4.16296600 -0.46347000  H -3.56125200 3.38704500 0.09943100  C -0.91520300 -0.48466900 -1.18238900  O -1.50867300 -1.00212700 -2.08212400  O -0.77768600 -1.06051300 0.08954300  C -1.47603100 -2.20517700 0.40193700  F -2.79065400 -2.07752900 0.24497800  F -1.05159100 -3.25770800 -0.32207400  F -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)