Supporting Material

Dynamics of nuclear recoil: QM-BOMD simulations of model systems following β-decay

Rasmus Fromsejer,[a] Kurt V. Mikkelsen[a] and Lars Hemmingsen[a]

[a]Department of Chemistry, University of Copenhagen, Universitetsparken 5, 2100 København Ø, Denmark. E-mail: rf@chem.ku.dk, kmi@chem.ku.dk, lhe@chem.ku.dk

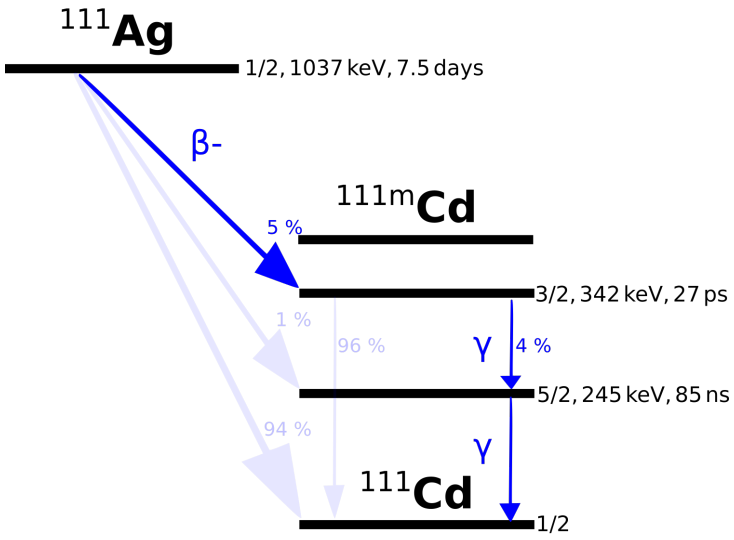

Figure S1: Decay scheme of ^{111}Ag. The dark blue arrows indicate the decay pathway used in ^{111}Ag γ-γ perturbed angular correlation spectroscopy. The nuclear spin, energy and half-life of relevant energy levels and percentage probability of relevant pathways is shown.

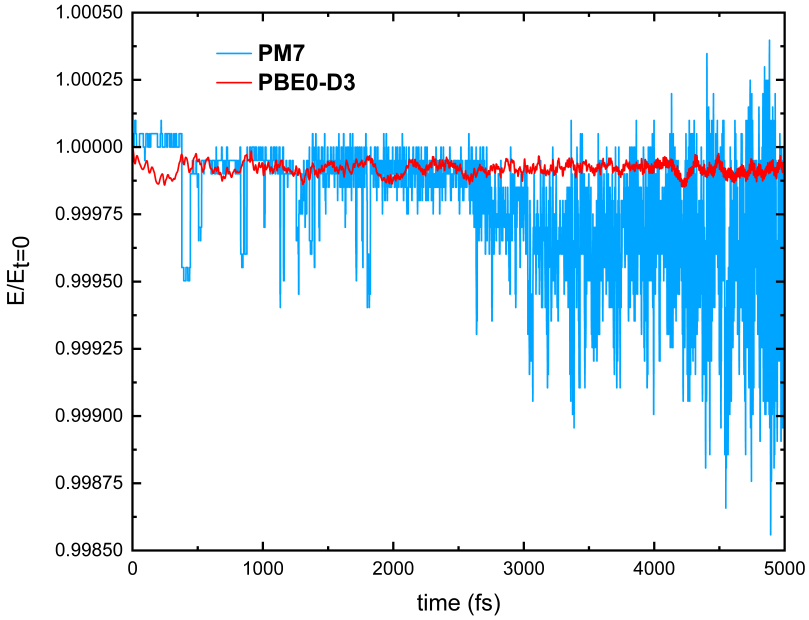

Figure S2: Trajectory of the ratio of the total energy E relative to the start energy E_0 for the PBE0-D3-MD and PM7-MD simulations. $E_{rec} = 500$ kJ/mol, $\Delta t = 0.5$ fs, $E_{therm} = 0$.

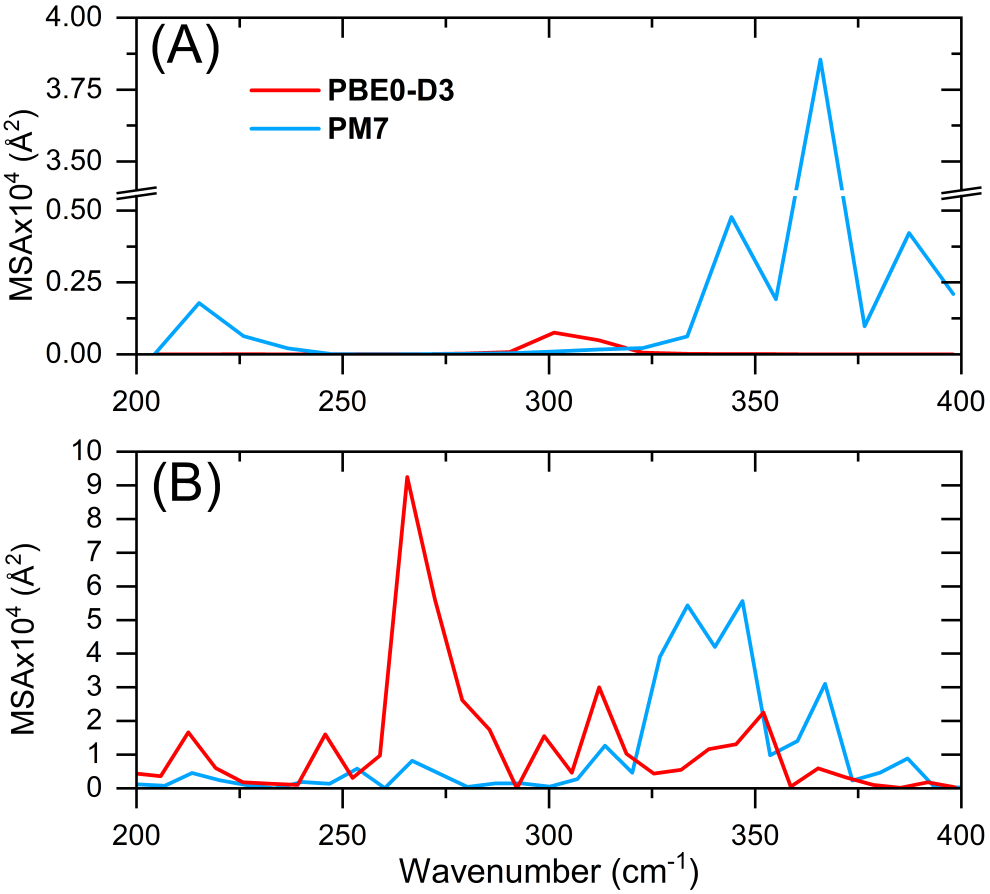

Figure S3: Comparison of power spectral data as function of wavenumber for the Cd-S4 bond from the PBE0-D3-MD and PM7-MD simulations of model 1: (A) E_{rec} = 0 kJ/mol trajectories, (B) E_{rec} = 500 kJ/mol trajectories. Δt = 0.5 fs, E_{therm} = 0 kJ/mol.

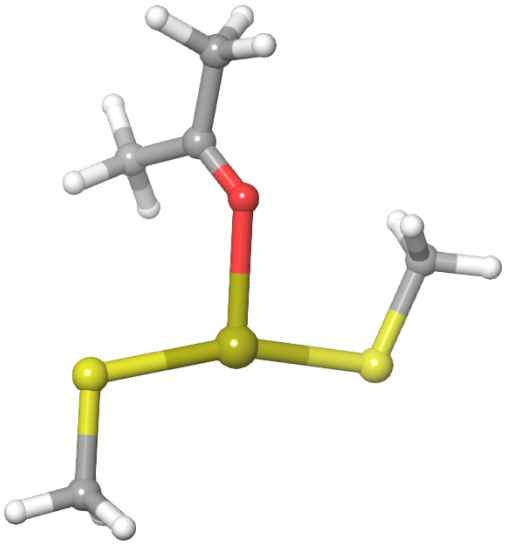

Figure S4: PM7 optimized structure of acetone-model 1 interaction.

Method	r(Cd-O)
PM7	2.33
PM6	3.34
PBE0-D3	2.53
CAM-B3LYP	2.50
ωB97XD	2.51
M062X	2.46

Table S4: Cadmium-carbonyl oxygen bond-lengths (in Ångström) in optimized structures of acetone-model 1 interaction. The def2-TZVP basis-set was used for the DFT calculations.

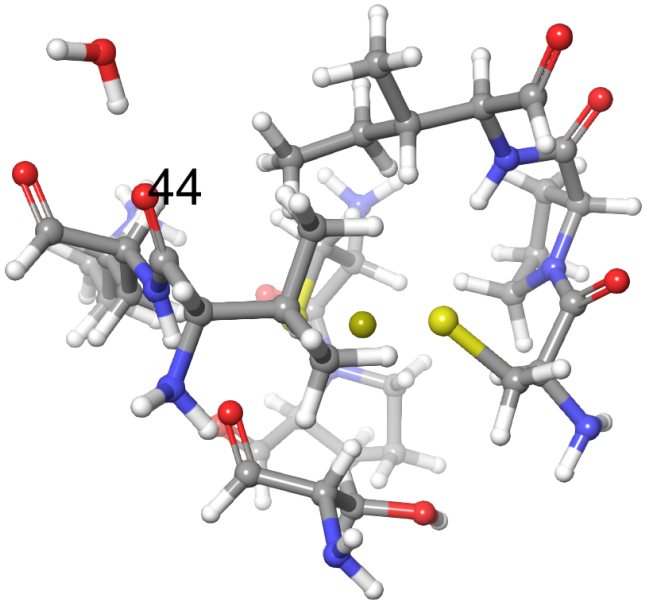

Figure S5: Model 2 structure with additional water acting as hydrogen bond donor. Hydrogen bond distance 1.75 Å.

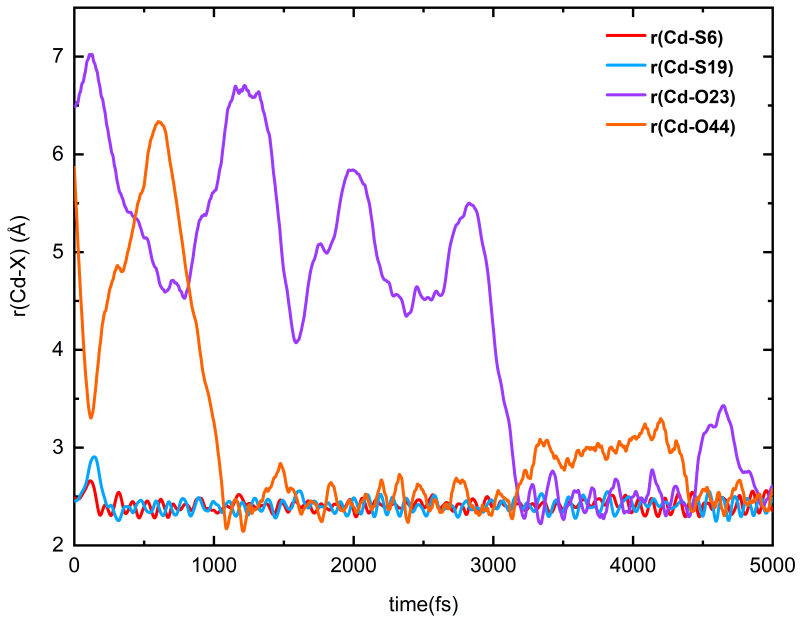

Figure S6: PM7-MD trajectories of selected inter-atomic distances in model 2 with additional water acting as hydrogen bond donor (non-frozen) (fig. S4). Recoil perpendicular to S-Cd-S plane, E_{rec} = 500 kJ/mol. E_{therm} = 0, Δt = 0.5 fs.

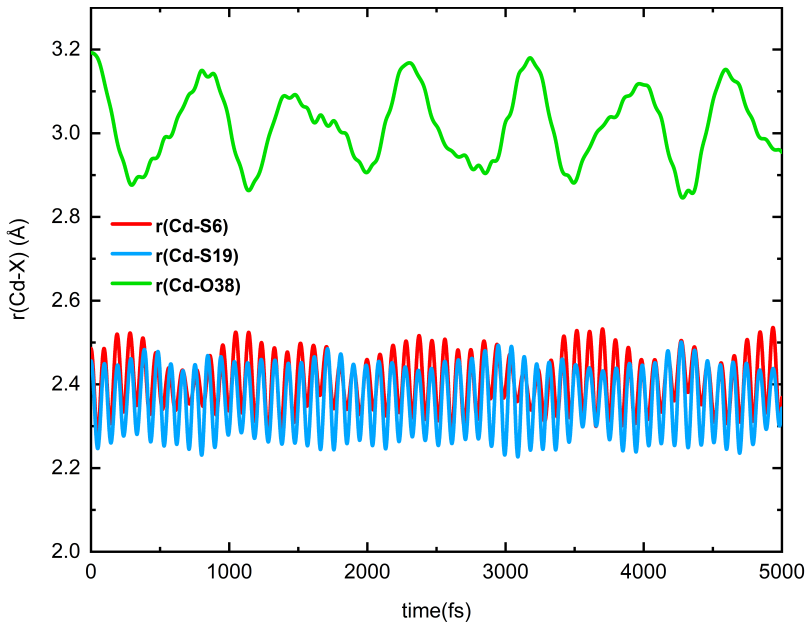

Figure S7: PM7-MD trajectories of selected inter-atomic distances in model 2 (frozen). E_{rec} = 0 kJ/mol, E_{therm} = 0, Δt = 0.5 fs.

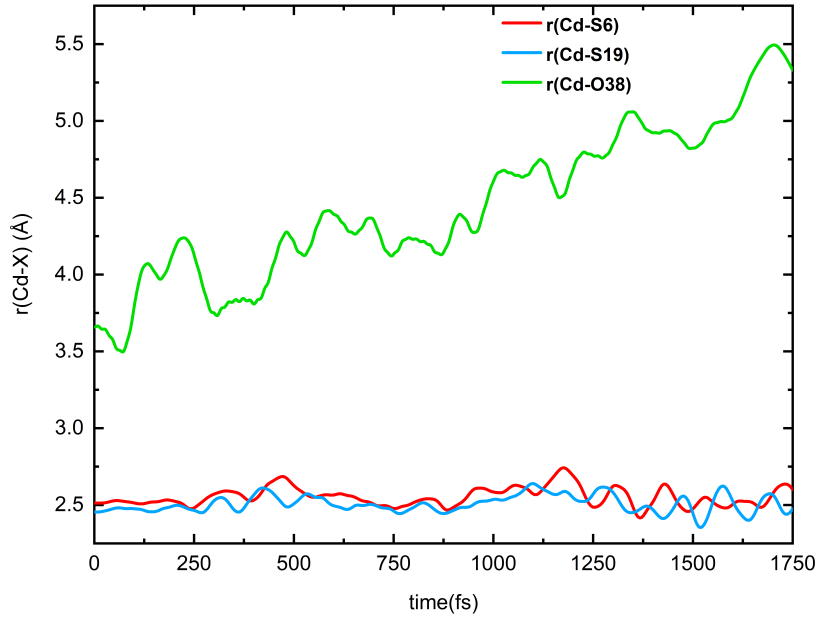

Figure S8: PM7-MD trajectories of selected inter-atomic distances in model 3 (non-frozen) with ^{111}Ag(I) occupying metal-site. E_{rec} = 0 kJ/mol, E_{therm} = 0, Δt = 0.5 fs.

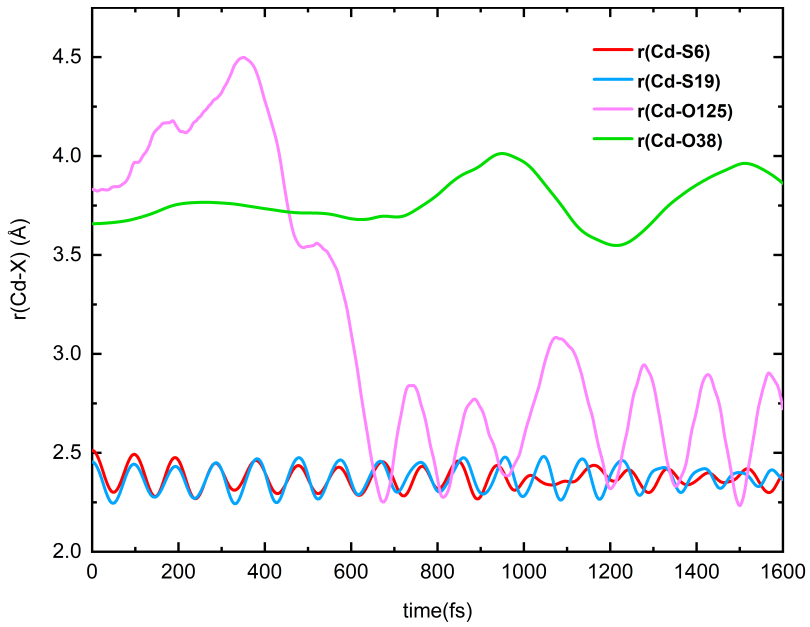

Figure S9: PM7-MD trajectories of selected inter-atomic distances in model 3 (frozen). E_{rec} = 0 kJ/mol, E_{therm} = 0, Δt = 0.5 fs.

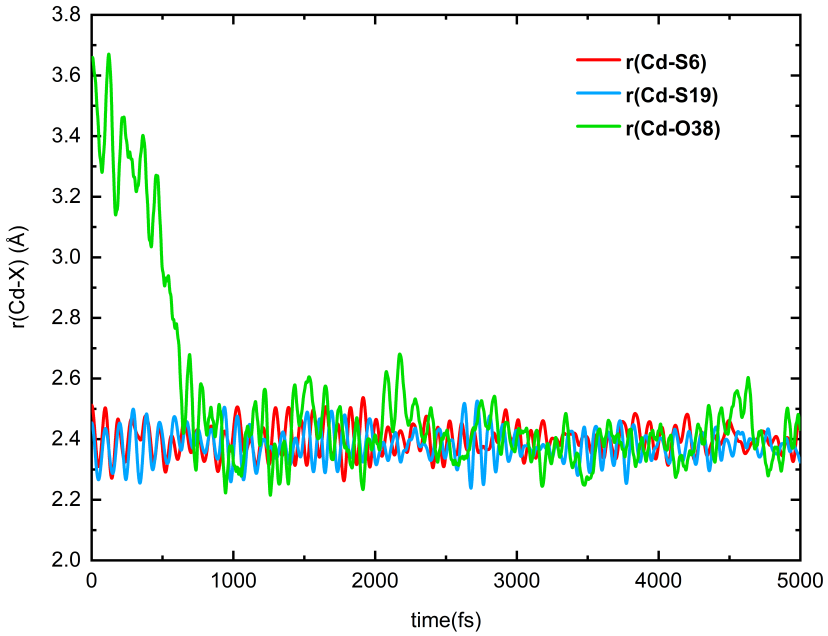

Figure S10: PM7-MD trajectories of selected inter-atomic distances in model 3 (non-frozen). E_{rec} = 0 kJ/mol, E_{therm} = 0, Δt = 0.5 fs.

```
11
Model 1 Cartesian coordinates in Bohr optimized with PBE0
C 139.269436 39.71156743 152.2386652
S 142.0145635 41.52114447 151.2296157
C 149.3805925 36.2529399 145.9639661
S 146.1495428 36.77231408 144.9059463
Cd(Iso=111) 144.1057683 39.03239424 148.1690571
H 138.0676421 40.93262521 153.3974149
H 138.1475907 39.05409774 150.6364515
H 150.4821762 35.51933693 144.3745308
H 150.2737829 38.000447 146.6013593
H 149.4916858 34.87337568 147.4976337
H 139.7883037 38.07060875 153.381305


11
Model 1 Cartesian coordinates in Bohr optimized with PM7
C 139.6919466 39.01566071 151.5537566
S 142.2281479 41.33473245 151.2810692
C 150.0355508 35.92047852 145.8093676
S 147.3366441 37.5605717 144.4514105
Cd(Iso=111) 144.9278104 39.62377454 147.8396892
H 137.8982187 40.0599233 151.3799019
H 139.6966709 37.60913766 150.0177874
H 150.7959765 34.6309295 144.3336806
H 151.558292 37.27881356 146.2296426
H 149.4916876 34.87338135 147.4976488
H 139.7883226 38.07060875 153.3813107


125
Model 2 Cartesian coordinates in Bohr partially optimized with PM7
N 137.4147947 36.2608314 154.4250914
C 139.7781956 37.65588381 154.1499926
C 140.2325197 39.74853236 156.0819256
O 138.4961186 41.1261067 156.7735445
C 139.6919674 39.01575331 151.5537377
S 142.228146 41.33473812 151.2811164
N 142.6062669 39.99792328 156.9738744
```

```
C 143.4018472 41.90844948 158.81823
C 144.5526904 44.23092272 157.5067601
O 143.3886191 45.35908913 155.8400218
C 145.3369247 40.48737553 160.3942614
C 146.6786302 38.99449389 158.4157183
C 144.5186734 37.97593159 156.7981129
N 151.722409 33.49524765 149.312587
C 149.3646697 34.38026113 148.1811305
C 147.6447602 32.20243129 147.394859
O 148.178997 30.86687312 145.5636031
C 150.0354676 35.92039915 145.8094545
S 147.3366933 37.56056981 144.4514388
N 145.5447889 31.8211016 148.7781082
C 143.7098726 29.81042559 148.2471028
C 142.4664329 30.11845092 145.6695165
O 141.6765274 28.27407836 144.4903275
C 141.7842418 30.09577421 150.3862726
C 143.3281479 31.13701323 152.4989862
C 144.9306337 33.09476936 151.1761781
N 142.2850192 32.46738033 144.8059136
C 141.0888226 33.01540086 142.3851746
C 142.5609192 31.91935979 140.1609672
O 141.5366877 30.47938859 138.6472966
C 140.7770178 35.88967409 142.0280164
C 139.3238185 36.98760489 144.2843493
C 139.3616131 36.428246 139.5657035
C 139.1386254 39.85053788 144.307026
N 152.6331568 44.23848162 147.8238042
C 150.0952548 43.58085698 148.67985
C 148.245213 45.79561584 148.6193788
O 146.1230508 45.53483365 147.6990822
C 150.2029692 42.48103645 151.3462534
O 151.5616822 40.18123992 151.3405842
N 146.8260288 47.60786306 141.3722815
C 145.1876364 45.78427748 140.1175035
C 142.4834404 46.00915487 141.1190582
O 140.6541856 45.80317474 139.6866459
C 146.1362788 43.05551315 140.5181254
C 144.3467102 41.19224333 139.2425603
C 148.7856747 42.77205426 139.4390918
```

```
N 142.2528938 46.43434322 143.5832609
C 139.7943603 46.71591239 144.7907958
C 138.4753316 49.02893701 143.6796369
O 136.2001015 49.00437057 143.203426
C 140.1231726 47.0579528 147.6480596
C 137.6684186 47.03716581 149.1220459
C 138.1181734 47.56061991 151.9056123
C 135.6539707 47.51526649 153.3795986
N 134.5012378 44.95090832 153.3739294
Cd(Iso=111) 144.927818 39.62373863 147.8396854
H 135.7887459 37.08839343 153.8666698
H 141.319681 36.30326897 154.3302082
H 137.8982338 40.05990062 151.3799113
H 139.6966142 37.60921892 150.0178176
H 141.8054067 42.47253269 159.9911829
H 144.3567258 39.19707252 161.665858
H 146.6502843 41.83645092 161.2297093
H 147.6633664 37.41865139 159.3046454
H 147.8394889 40.26098636 157.2794261
H 145.1528673 37.80887981 154.845459
H 143.7743122 36.26024936 157.6613397
H 152.7965463 34.99526867 149.8015536
H 151.3328363 32.45943025 150.8679562
H 148.3685498 35.52242852 149.574709
H 150.7960313 34.63089549 144.3336881
H 151.5582296 37.2788986 146.2297277
H 144.6282775 27.97077734 148.3689901
H 141.0752166 28.23552795 150.9152069
H 140.3603332 31.47980953 149.838819
H 144.5473991 29.65301141 153.2431603
H 142.08622 32.07601807 153.8476837
H 143.7814932 34.75867309 150.7846268
H 146.6635124 33.38975558 152.2499204
H 142.9834619 33.91774502 145.8312771
H 139.2128916 32.16464622 142.3917887
H 142.6404766 36.76291647 141.9380655
H 140.1981948 36.34679881 146.0357454
H 137.4289903 36.18125881 144.3329152
H 139.148452 38.46291397 139.3260862
H 140.4255288 35.65874958 137.9787116
```

H 137.5009889 35.54744472 139.6354344
H 138.0813237 40.45808478 145.9671484
H 141.031186 40.66160827 144.3648497
H 138.1701408 40.4903991 142.6055167
H 154.1307646 43.48996116 148.7401323
H 149.3673323 42.11858701 147.425072
H 148.2882988 42.14504317 152.0276886
H 151.1300687 43.82255293 152.6048109
H 151.617807 39.50698569 153.0237632
H 148.3578407 46.97499383 142.3188453
H 145.1776208 46.1883009 138.0977643
H 146.190136 42.65564713 142.5380535
H 145.03098 39.27152772 139.5350899
H 142.4637872 41.38064901 140.0560874
H 144.2641292 41.59059757 137.2233881
H 149.4431104 40.84151019 139.7285978
H 148.7552501 43.19081753 137.4225652
H 150.0597279 44.08031156 140.3918917
H 143.810406 46.57134836 144.6777902
H 138.6563673 45.03783572 144.4279684
H 141.1241605 48.82050023 148.0139106
H 141.3673682 45.58528934 148.3731475
H 136.7556809 45.20299777 148.9081289
H 136.3951212 48.46220818 148.3534943
H 139.0122027 49.40366967 152.1210411
H 139.4012973 46.14294747 152.6713293
H 134.334186 48.86188523 152.5503868
H 136.0058377 48.10429408 155.32167
H 135.6131526 43.7503654 154.3563979
H 132.7753511 45.02649736 154.1853777
H 134.3315404 44.33258998 151.576233
H 137.507482 34.64652541 153.4092219
H 146.4085884 44.86946113 158.066119
H 144.5249095 32.42108204 139.9232396
H 152.8544437 43.69291773 146.0083444
H 148.8085404 47.59935929 149.390576
H 147.5295738 48.82560249 140.0819766
H 139.5766639 50.70739163 143.3120852

138

```
Model 3 in Cartesian coordinates in Bohr partially optimized with PM7
N -23.591339 35.199926 1.241550
C -24.360458 32.595884 0.589595
C -24.400142 32.055422 -2.326253
O -23.965505 29.916252 -3.259777
C -26.956941 32.206600 1.891616
O -29.084773 33.591769 1.071475
H -24.880132 36.256283 2.169405
H -23.219063 31.295752 1.706423
H -26.781197 32.493838 3.923071
H -27.459608 30.269631 1.407846
H -29.226502 35.058197 2.131611
N -17.980743 29.075324 -3.972204
C -17.801219 26.516635 -3.163401
C -19.280874 24.991626 -5.109819
O -18.489079 23.056547 -5.962085
C -18.713956 25.938379 -0.453534
C -18.593014 23.160482 0.421409
C -17.111469 27.387799 1.547686
H -19.263867 30.228057 -3.152063
H -15.811337 26.013968 -3.348594
H -20.671713 26.548760 -0.257003
H -19.481185 21.977513 -1.012893
H -16.712737 22.342230 0.234326
H -19.481185 22.822221 2.248774
H -17.419494 29.394688 1.198086
H -17.557444 26.794425 3.469537
H -15.119698 27.138355 1.084703
N -21.675157 25.688935 -5.733429
C -23.355123 24.294317 -7.519220
C -22.211839 23.899365 -10.174285
O -22.315774 21.847122 -11.219303
C -25.959166 25.700273 -7.880157
C -27.722280 24.111014 -9.488314
C -30.570097 24.764859 -9.038559
C -32.476831 23.610237 -10.935844
N -35.084653 24.073219 -10.091137
H -22.521754 26.835999 -4.465423
H -23.948497 22.523644 -6.651835
H -25.775862 27.601338 -8.653055
```

```
H -26.716946 26.051762 -5.996101
H -27.433152 22.085228 -9.255878
H -27.418034 24.063771 -11.523549
H -30.674032 26.822771 -9.004544
H -30.819541 24.205500 -7.071355
H -32.446595 21.557994 -11.107809
H -32.078099 24.243295 -12.853916
H -36.237386 22.905369 -11.066235
H -35.027961 23.619685 -8.237316
H -35.235831 25.964835 -10.287668
N -35.686812 20.303817 -0.495358
C -34.388402 22.868717 -0.699592
C -35.632412 24.245908 -2.928172
O -35.346673 23.329094 -5.058895
C -31.610786 22.399740 -1.454205
S -29.870513 25.339111 -1.848041
H -34.771240 18.867128 -1.359184
H -34.490827 23.639803 1.204052
H -31.519326 21.371004 -3.277599
H -30.713917 21.138227 -0.052362
N -37.028842 26.363800 -2.556845
C -37.683026 28.173925 -4.471092
C -35.405906 29.262407 -5.928070
O -35.235831 29.201936 -8.258103
C -39.274175 30.241285 -3.212534
C -38.635448 30.133571 -0.349599
C -37.968375 27.325438 -0.120942
H -38.625999 27.452049 -6.152948
H -41.296182 29.852001 -3.165291
H -39.332757 32.166916 -3.941968
H -40.098096 30.895130 0.884392
H -36.879892 31.169140 -0.060471
H -36.728714 27.004184 1.494773
H -39.574642 26.104675 0.287238
N -33.722160 30.194042 -4.232986
C -31.569762 31.499843 -4.877383
H -34.015068 29.961606 -2.362157
H -30.348999 30.492619 -6.194522
H -30.392463 31.322208 -3.195527
C -29.666769 31.290115 9.718846
```

```
O -31.127566 31.518740 7.912283
N -28.077613 29.409815 9.966385
C -27.406964 27.642583 7.991719
C -27.922559 24.919919 9.006723
O -26.441008 23.889889 10.599420
C -24.582595 27.866249 7.397204
S -23.458357 25.706899 4.956322
H -27.083494 29.449554 11.595321
H -28.585736 28.171956 6.387138
H -23.450504 27.388623 9.103307
H -24.094923 29.822044 6.886018
N -29.963501 23.723624 8.222207
C -30.590884 21.026981 8.645496
C -28.551870 19.093791 8.055902
O -28.344000 17.328787 9.546896
C -33.128786 20.435497 7.131826
C -34.234276 23.092452 6.784116
C -31.911803 24.713836 6.462863
H -31.276855 20.883362 10.582466
H -34.629229 19.449060 8.140940
H -32.962490 19.407486 5.353594
H -35.182918 23.778422 8.479201
H -35.485275 23.152923 5.147614
H -31.639682 24.823441 4.423849
H -32.433367 26.578996 7.165841
N -26.962610 19.288433 6.043344
C -24.793205 17.685946 5.448080
C -22.814662 17.803109 7.591029
O -21.956726 15.903934 8.562348
C -23.642362 18.252863 2.983877
C -25.484845 17.967515 0.776677
C -21.151703 16.975409 2.271451
C -24.863125 19.728739 -1.559024
H -27.208275 20.974069 5.183518
H -25.539647 15.771653 5.295012
H -23.113239 20.240855 3.097261
H -27.401027 18.337901 1.438081
H -25.464058 15.917162 0.580146
H -21.429493 15.002535 1.749886
H -20.482740 17.927830 0.570697
```

```
H -19.783541 17.011313 3.811577
H -23.631023 21.319889 -1.126277
H -23.770863 18.806553 -3.042459
H -26.694269 20.401482 -2.224207
Cd(Iso=111) -26.381493 25.388291 1.370994
O -32.537302 29.196267 1.547686
H -31.148353 30.348999 1.642172
H -31.864560 27.743067 0.706758
O -35.524959 31.237171 4.875493
H -34.139790 31.441261 6.018777
H -34.789855 30.505847 3.395838
H -29.656226 32.687913 11.205886
H -31.928999 33.453252 -5.423325
H -24.827409 33.633910 -3.547205
H -22.194832 19.642001 8.223332
H -22.050646 35.146258 2.366882
H -16.309280 29.951968 -3.688556
H -35.850808 19.818807 1.343555
H -21.309684 25.474829 -11.106676
```