SUPPORTING INFORMATION

Title: Structural and Energetical Characterization of the Methylbutadiene–Fe(CO)$_3$ Isomers and Related Reactive Intermediates with Quantum Chemical Methods
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Ref. No.: I99146

xyz coordinates of structure 1

```
 6  0.118832  -1.602850   1.375592
 6 -1.149719  -1.578566   0.710477
 6 -1.149719  -1.578566  -0.710477
 6  0.118832  -1.602850  -1.375592
26 -0.004522   0.012214   0.000000
 6 -0.513803   1.151956   1.296349
 6 -0.513803   1.151956  -1.296349
 6  1.768357   0.243167   0.000000
 8 -0.826319   1.870020   2.149222
 8 -0.826319   1.870020  -2.149222
 8  2.920797   0.358216   0.000000
 1  0.899422  -2.280806   1.038127
 1 -2.078392  -1.407368   1.251935
 1 -2.078392  -1.407368  -1.251935
 1  0.128188  -1.416376  -2.448092
 1  0.128188  -1.416376   2.448092
 1  0.899422  -2.280806  -1.038127
```

xyz coordinates of structure 2

```
 6  1.190782   -.695329  -1.402765
 6  1.757471   -.618157   -.085183
 6  1.053816  -1.322799    .931360
 6  -.134671  -2.039234    .570196
26  -.260007   -.014268   -.017082
 6   .093624   1.708883   -.390393
 6 -1.155367    .417904   1.481988
 6 -1.607798   -.350738  -1.142111
 8   .328009   2.811216   -.658841
 8 -1.741204    .670433   2.448632
 8 -2.464508   -.599562  -1.881014
 1   .848979  -1.647684  -1.802262
 1  1.343223  -1.189282   1.973056
 1  -.756175  -2.415137   1.381247
 1  1.598163   -.025304  -2.159538
 1  -.145802  -2.666905   -.318411
 6  2.970162    .225703    .233012
 1  2.971712    .565865   1.275450
 1  3.032983   1.103252   -.420573
 1  3.880612   -.367924    .068324
```

xyz coordinates of structure 2'

```
 6  1.196409    .183955  -1.628867
 6  1.778978   -.351940   -.446951
 6  1.166336  -1.545026    .074135
 6   .050790  -2.098434   -.609357
26  -.261951   -.030810   -.028456
 6  -.023600    .595059   1.635220
 6 -1.899976   -.686589    .130672
 6  -.839617   1.447410   -.813326
 8   .100011   1.014005   2.709936
 8 -2.973229  -1.116233    .248446
 8 -1.206104   2.426541  -1.320646
 1   .825786   -.452051  -2.428042
 1  1.496078  -1.944793   1.031558
 1  -.488611  -2.905976   -.118775
 1  1.542635   1.161901  -1.960271
 1  -.000097  -2.116981  -1.694929
 6  2.950446    .300262    .249811
 1  2.957842    .090639   1.325873
 1  2.942693   1.387021    .108446
 1  3.890375   -.081387   -.173912
```

xyz coordinates of structure 3

```
 6 -1.785010   -.709891   -.011755
 6 -1.106793  -1.009305  -1.232228
 6   .120892  -1.724870  -1.170865
 6   .610628  -2.101733    .122087
26   .266229   -.012746   -.006830
 6  -.178897   1.636057   -.568564
 6  2.000686    .282361   -.370761
 6   .223427    .184439   1.768069
 8  -.470497   2.703244   -.913041
 8  3.127112    .448492   -.584009
 8   .184035    .286171   2.922124
 1 -1.798701  -1.480550    .757270
 1 -1.433041   -.575224  -2.177049
 1   .721974  -1.844414  -2.070107
 1  1.626169  -2.489365    .180750
 1  -.064557  -2.527247    .861320
 6 -3.003295    .190527   -.001184
 1 -2.957355    .957162   -.784006
 1 -3.113232    .701504    .962884
 1 -3.918244   -.399236   -.162869
```

xyz coordinates of structure 4

```
 6 -1.710951   0.558444  -0.642468
 6 -1.040165  -0.259083  -1.623034
 6 -0.497794  -1.518774  -1.253998
 6 -0.577661  -1.961971   0.106721
26  0.264559  -0.015051  -0.018976
 6  0.908504   1.568535  -0.576119
 6  1.925553  -0.707232   0.087693
 6 -0.104504   0.341850   1.689359
 8  1.305495   2.598322  -0.927893
 8  2.983601  -1.168713   0.181649
 8 -0.387004   0.563660   2.791360
 1 -0.777869   0.144325  -2.600955
 1  0.143610  -2.036467  -1.966318
 1  0.053905  -2.805181   0.383077
 1 -1.500994  -1.909001   0.668711
 1 -1.765093   1.607890  -0.942464
 6 -2.959456   0.172758   0.143297
 1 -3.845695   0.483211  -0.430274
 1 -3.000814   0.692491   1.108285
 1 -3.063475  -0.899252   0.323688
```

xyz coordinates of structure 5

```
 6 -1.057184  -0.471780  -1.750540
 6 -1.563112  -1.007743  -0.527921
 6 -2.091013  -0.055348   0.465507
 6 -2.023445   1.306886   0.279360
26  0.058763   0.009330   0.017142
 6  1.553972  -0.817448  -0.605332
 6  0.667412   0.054773   1.768046
 6  0.664701   1.630505  -0.580396
 8  2.488940  -1.340786  -1.007352
 8  1.038797   0.079817   2.849501
 8  1.063150   2.626701  -0.980121
 1 -1.554453   0.367163  -2.230158
 1 -2.348078  -0.445285   1.449265
 1 -2.200058   1.971748   1.123193
 1 -0.544311  -1.142928  -2.436047
 1 -1.976260   1.771904  -0.700052
 6 -0.856114  -2.062640   0.093744
 1 -1.111552  -2.380181   1.101832
 1 -0.291526  -2.774078  -0.504769
```

xyz coordinates of structure 5'

```
 6 -1.147912    .836226  -1.394458
 6 -1.600392   -.399361   -.860934
 6 -2.638023   -.498176    .185806
 6 -3.514195    .476755    .509910
26   .372453    .066850   -.113486
 6  1.949838   -.612664   -.653582
 6   .628421   -.786340   1.467664
 6   .997700   1.764947    .315428
 8  2.934120  -1.030023  -1.063981
 8   .716023  -1.301937   2.485728
 8  1.402694   2.800258    .578978
 1 -1.653228   1.776252  -1.190404
 1 -2.718097  -1.466407    .680818
 1 -4.279306    .303505   1.263632
 1  -.558608    .820075  -2.316872
 1 -3.517802   1.454050    .030052
 6  -.722047  -1.503379  -1.062764
 1  -.914902  -2.447381   -.556912
 1  -.184877  -1.592623  -2.007890
```

xyz coordinates of structure 5ts

```
 6  1.530213  -0.076891  -1.333858
 6  1.821876  -0.376078   0.080989
 6  1.174731  -1.495525   0.683631
 6  0.179810  -2.158309  -0.065039
26 -0.173683  -0.022239  -0.009429
 6 -0.132541   1.806950   0.041983
 6 -1.338424  -0.126191   1.409639
 6 -1.473837  -0.190526  -1.277907
 8 -0.109572   2.953278   0.061842
 8 -2.053305  -0.209356   2.300298
 8 -2.248742  -0.316433  -2.112184
 1  1.594998  -0.883710  -2.068763
 1  1.340362  -1.708301   1.739146
 1 -0.440095  -2.888340   0.450914
 1  1.800330   0.903066  -1.728254
 1  0.287038  -2.324626  -1.134744
 6  2.966911   0.386701   0.451098
 1  3.922123   0.149449  -0.021588
 1  2.931531   1.289971   1.065591
```

xyz coordinates of structure 6

```
6 -1.075708   0.913526  -1.242249
6 -1.562115  -0.367811  -0.810994
6 -2.661708  -0.553366   0.159443
6 -3.639892   0.354690   0.383896
26  0.547613  -0.005390  -0.288741
6  1.456437   1.588439  -0.202104
6  1.879524  -1.241327   0.001950
6  0.148157   0.069336   1.450811
8  2.017965   2.606607  -0.186262
8  2.716078  -2.035026   0.150896
8 -0.141423   0.111404   2.577235
1 -1.540885   1.831492  -0.897055
1 -2.708817  -1.524308   0.651234
1 -4.455491   0.135405   1.067194
1 -0.621869   0.992111  -2.237202
1 -3.678724   1.319365  -0.118088
6 -0.696502  -1.458871  -1.145513
1 -0.880822  -2.453796  -0.750621
1 -0.181454  -1.451709  -2.114587
```

xyz coordinates of structure 6'

```
6  .996882  -1.201965  -1.058542
6  1.613457  -.000027   -.619632
6  2.656273  -.000004   .456546
6  3.961335  .000000   .151487
26  -.529130  .000009   -.294056
6 -1.694170  -1.444814  -.216538
6 -1.694055   1.444924  -.216451
6  -.358505  -.000074   1.491752
8 -2.399519  -2.343028  -.191850
8 -2.399330   2.343193  -.191689
8  -.232020  -.000124   2.629346
1  1.314937  -2.163706  -.662877
1  2.342857   .000008   1.500501
1  4.713366   .000014   .937435
1  .564700  -1.240421  -2.067955
1  4.320011  -.000012   -.877122
6  .996913   1.201896  -1.058611
1  1.314994   2.163661  -.663024
1  .564693   1.240288  -2.068013
```

xyz coordinates of structure 9

```
6 -0.655742  -1.374935  -1.355161
6 -0.972545  -1.515483   0.038159
6 -1.753230  -0.467029   0.638320
26  0.269273  -0.004025  -0.000869
6  1.925688  -0.257423  -0.653155
6  0.697660   0.795614   1.549976
6 -0.177934   1.461228  -0.939604
8  2.987177  -0.442954  -1.074603
8  0.961004   1.293526   2.561090
8 -0.483630   2.396264  -1.549356
1 -1.380887  -0.944930  -2.041227
1 -1.798884  -0.500726   1.728480
1  0.028163  -2.091416  -1.805976
6  0.140115  -1.949382   0.840296
1  0.033356  -1.982183   1.923301
```

```
1  0.840438  -2.670540   0.423723
6 -2.964203   0.184117   0.004661
1 -2.893314   0.260191  -1.085128
1 -3.115316   1.195008   0.402015
1 -3.869916  -0.395688   0.239417
```

xyz coordinates of structure 11

```
6 -2.122985   -.522391    .130430
6 -1.443485   -.876872  -1.130593
6  -.409637  -1.830580  -1.013505
6   .085562  -2.150176    .288822
26   .074119   -.017353    .016893
6  -.014569   1.701110   -.667755
6  1.755188   -.132723   -.652768
6  .675632    .266864   1.728309
8  .004174   2.760728  -1.102599
8  2.814924   -.223200  -1.076034
8  1.017717    .420661   2.809671
1 -2.299702  -1.309191    .861733
1 -1.781181   -.501435  -2.094041
1  .146127  -2.120127  -1.904562
1  1.026759  -2.693199    .347777
1  -.586335  -2.355518   1.117592
6 -2.486258    .749723    .475245
1 -2.901280    .954810   1.461126
1 -2.462693   1.580600   -.226261
```

xyz coordinates of structure 11ts

```
6 -1.783295  -0.376466   0.006355
6 -1.176954  -1.074256  -1.164551
6 -0.128570  -1.954234  -0.821273
6  0.221462  -2.104698   0.549123
26  0.169774  -0.014708  -0.017295
6 -0.064872   1.637534  -0.746226
6  1.947730  -0.011504  -0.522743
6  0.421572   0.468430   1.712530
8 -0.248655   2.678410  -1.195924
8  3.050841  -0.026447  -0.831843
8  0.525204   0.745886   2.821783
1 -2.190945  -1.224875   0.655794
1 -1.518493  -0.900592  -2.182070
1  0.503402  -2.341857  -1.619542
1  1.170896  -2.578250   0.789383
1 -0.549031  -2.259441   1.303020
6 -3.005243   0.311431   0.108279
1 -3.954617  -0.190947  -0.110315
1 -3.085447   1.318162   0.532306
```

xyz coordinates of structure 12

```
6 -1.610408   1.263022   -.608546
6 -1.710965   -.002015  -1.267422
6 -1.605319  -1.267998   -.611401
6 -1.448679  -1.467064    .773103
26   .036081    .000075   -.005059
6  1.145296   1.288317   -.705175
6  1.150572  -1.283791   -.704567
6   .733436    .001194   1.672808
```

```
8  1.841646   2.090726  -1.129406
8  1.850121  -2.083772  -1.128122
8  1.152033    .001818   2.738920
1 -1.743318   -.000837  -2.355032
1 -1.426389  -2.116684  -1.272730
1 -1.119382  -2.453948   1.093166
1 -2.012400   -.920361   1.515896
6 -1.455005   1.459902    .776305
1 -1.434687   2.113841  -1.267993
1 -1.129697   2.447408   1.098521
1 -2.016205    .909032   1.517927
```

xyz coordinates of structure 13

```
6 -2.108579   0.488772   0.208140
6 -1.498562   0.287051  -1.139711
6 -0.959991  -0.982375  -1.443424
6 -0.684091  -1.892315  -0.382537
26  0.194108   0.008579   0.040276
6  0.668746   1.811138   0.090352
6  1.688143  -0.354038  -0.904757
6  0.934243  -0.636434   1.603764
8  0.994958   2.906536   0.100516
8  2.623873  -0.598229  -1.516690
8  1.357739  -1.054894   2.579780
1 -1.620838   1.040930  -1.916325
1 -0.539475  -1.147709  -2.435500
1 -0.066091  -2.761505  -0.598162
1 -1.398042  -2.024225   0.426020
6 -3.364025   0.189063   0.586417
1 -1.491166   1.000558   0.980577
1 -3.711294   0.391839   1.597579
1 -4.087772  -0.215422  -0.119677
```

xyz coordinates of structure 14

```
6  1.326747   1.197728   0.490987
6  2.127450   0.265658  -0.362330
6  1.185765  -0.252278  -1.372891
6  0.198309   0.635963  -1.906851
26 -0.369666   0.017849   0.007334
6  0.006102  -0.962580   1.440605
6 -1.567562  -1.106076  -0.667199
6 -1.433524   1.352518   0.480827
8  0.240338  -1.578151   2.411258
8 -2.351479  -1.847659  -1.128213
8 -2.095543   2.264014   0.812843
1  1.182665   2.198742   0.066232
1  1.371955  -1.218980  -1.845213
1 -0.395223   0.285691  -2.752484
1  1.688264   1.281804   1.521822
1  0.367543   1.712648  -1.905001
6  3.372168  -0.220522  -0.113601
1  3.797592  -1.026689  -0.713409
1  3.959253   0.134603   0.732977
```

xyz coordinates of structure 14ts

```
6  1.284146  -0.862152  -1.214720
6  1.851217  -0.558065   0.087917
```

6 1.075653 -1.113833 1.156460
6 -0.092199 -1.910235 0.878876
26 -0.269122 -0.018923 -0.013413
6 0.150993 1.638487 -0.558172
6 -1.240393 0.579058 1.350286
6 -1.489479 -0.539002 -1.183898
8 0.381736 2.720230 -0.922544
8 -1.910396 0.942331 2.235676
8 -2.301903 -0.893554 -1.948417
1 0.964247 -1.875177 -1.482741
1 1.340187 -0.799089 2.164423
1 -0.723968 -2.184186 1.725579
1 1.694154 -0.299253 -2.053205
1 -0.062731 -2.670259 0.097785
6 3.053105 0.292533 0.363428
1 3.901839 -0.240275 -0.114856
1 2.969671 1.247433 -0.187039

xyz coordinates of structure 15

6 .868245 -1.470598 .806376
6 1.312829 -.888474 -.430828
6 2.483641 -.014202 -.574582
6 3.571676 .035256 .229288
26 -.464352 -.027854 .010663
6 -1.984941 -.921353 .213795
6 -.837735 1.303049 -1.087884
6 -.280920 1.008379 1.432910
8 -3.013409 -1.473811 .363036
8 -1.095561 2.167054 -1.845335
8 -.159386 1.675816 2.393740
1 1.412044 -1.233474 1.721420
1 2.462264 .635521 -1.454856
1 4.380417 .740164 .040743
1 .420895 -2.465446 .794908
1 3.659495 -.599693 1.110083
6 .417519 -1.139147 -1.533352
1 .624220 -.658310 -2.491820
1 -.041223 -2.124488 -1.623571

xyz coordinates of structure 16

6 1.178424 .095646 -1.188335
6 2.256697 .202916 -.164172
6 2.564597 -.964978 .693923
6 1.919372 -2.150576 .700449
26 -.564273 .044958 -.038776
6 -.736603 1.794801 -.087390
6 -1.728822 -.162538 1.271182
6 -1.352424 -1.120696 -1.085746
8 -1.000641 2.930113 -.273471
8 -2.458098 -.322662 2.181550
8 -1.984817 -1.730985 -1.876684
1 1.284006 -.827590 -1.771990
1 3.404822 -.829544 1.382355
1 2.216297 -2.948937 1.380717
1 1.219682 .948289 -1.875615
1 1.061337 -2.333580 .056025
6 2.982239 1.335060 .065192

1 3.716710 1.391068 .869743
1 2.815822 2.241844 -.514830

xyz coordinates of structure 17

6 -2.556472 -0.324854 -0.182112
6 -1.443352 0.050483 -1.053914
6 -0.473847 -0.865397 -1.579615
6 -0.014002 -1.944826 -0.758949
26 0.471297 -0.023268 -0.001239
6 0.594306 1.735043 -0.071934
6 2.192655 -0.261027 -0.281485
6 0.108516 -0.382303 1.703586
8 0.652396 2.909872 -0.120277
8 3.345078 -0.443585 -0.451139
8 -0.024362 -0.612274 2.849849
1 -2.456593 -1.271204 0.353018
1 -1.627781 0.946845 -1.651441
1 -0.005823 -0.659409 -2.540981
1 0.779602 -2.579942 -1.153255
1 -0.705259 -2.466907 -0.099284
6 -3.692345 0.391974 0.006296
1 -3.846501 1.353099 -0.485961
1 -4.469029 0.055823 0.691418

xyz coordinates of structure 17ts

6 -1.837048 -0.615090 -0.297167
6 -1.019223 -0.728102 -1.477725
6 0.166411 -1.518319 -1.461717
6 0.541958 -2.163354 -0.232318
26 0.247892 -0.079261 0.014712
6 -0.309392 1.663081 -0.369082
6 1.955825 0.368244 -0.141949
6 -0.049477 -0.206672 1.751737
8 -0.260087 2.819941 -0.544079
8 3.095396 0.642554 -0.195605
8 -0.233891 -0.330392 2.901307
1 -2.051235 -1.585845 0.187747
1 -1.214191 -0.057608 -2.313993
1 0.845921 -1.483332 -2.313631
1 1.543706 -2.592013 -0.179019
1 -0.203806 -2.706270 0.345119
6 -2.754261 0.539673 -0.120260
1 -2.529769 1.153918 0.754711
1 -3.815912 0.238330 -0.065549

xyz coordinates of structure 18

6 -2.550898 .682190 -.133109
6 -1.341587 .637653 -.980146
6 -.752904 -.540994 -1.553457
6 -.634667 -1.705270 -.730935
26 .454547 -.026407 -.002417
6 1.210421 1.550019 -.234183
6 1.978404 -.892376 -.176153
6 -.010396 -.127649 1.713719
8 1.698355 2.612598 -.384644
8 2.986316 -1.493490 -.286911
8 -.228368 -.187540 2.867915

1 -1.186227 1.564583 -1.539520
1 -.257051 -.494084 -2.522576
1 -.085991 -2.559974 -1.128347
1 -1.420658 -1.960076 -.025745
1 -2.642105 1.594457 .465799
6 -3.554632 -.221174 -.037321
1 -4.385109 -.064218 .650948
1 -3.553962 -1.141051 -.619092

xyz coordinates of structure 19

6 -.839815 -.771254 -1.367389
6 -1.458607 -1.054316 -.107395
6 -2.725132 -.471497 .353365
6 -3.549514 .388285 -.290524
26 .474215 -.035838 -.001273
6 1.290050 -.995353 1.256432
6 -.181930 1.423939 .756256
6 1.753256 .857338 -.807304
8 1.875743 -1.559023 2.108976
8 -.595540 2.393302 1.278164
8 2.625072 1.425822 -1.360412
1 -1.254246 -.036009 -2.054491
1 -1.238627 -2.027517 .334617
1 -3.026737 -.787188 1.357255
1 -4.453932 .763203 .186779
1 -3.324613 .766650 -1.286795
6 .412385 -1.414062 -1.615694
1 .949129 -1.177675 -2.534521
1 .573073 -2.428972 -1.250035

xyz coordinates of structure 20

6 1.240123 -.052297 -1.499972
6 1.926722 -.370717 -.249604
6 1.280056 -1.430479 .498515
6 .213473 -2.155816 -.072318
26 -.219812 -.016437 -.006410
6 -.169324 1.790031 .010406
6 -1.067950 -.106925 1.589088
6 -1.593853 -.260865 -1.139362
8 -.147313 2.946187 -.021113
8 -1.612628 -.176373 2.608431
8 -2.461271 -.398584 -1.894186
1 1.058974 -.860415 -2.208828
1 1.555105 -1.581397 1.542009
1 -.337972 -2.844852 .564344
1 .192995 -2.393128 -1.131581
1 1.550762 .869185 -1.993173
6 2.960454 .395490 .320458
1 3.318888 .193423 1.327871
1 3.407880 1.224174 -.222316

xyz coordinates of structure 20ts

6 1.243786 -0.660401 -1.384461
6 1.799618 -0.566688 -0.053980
6 1.103255 -1.297785 0.952872
6 -0.063735 -2.038439 0.573231
26 -0.226576 -0.015364 -0.016505

6 0.077078   1.712511 -0.412232
6 -1.133257   0.412198   1.479989
6 -1.564037 -0.396821 -1.139408
8 0.280588   2.818199 -0.689905
8 -1.725658   0.663048   2.442485
8 -2.411303 -0.675786 -1.877946
1 0.948592 -1.628940 -1.785140
1 1.380734 -1.160307   1.996572
1 -0.685592 -2.430872   1.376152
1 -0.051224 -2.661660 -0.318352
1 1.644223   0.019768 -2.134880
6 2.976500   0.275572   0.259016
1 3.970305 -0.164316   0.189185
1 2.899687   1.341200   0.458359

xyz coordinates of structure 21

6 -1.066268   0.660856 -1.457513
6 -1.486667 -0.534028 -0.809401
6 -2.536481 -0.530576   0.237734
6 -3.533173   0.368475   0.351747
26 0.346412 -0.002450   0.020866
6 1.840331   0.000981 -1.061399
6 1.033061 -0.992232   1.365446
6 0.564151   1.645947   0.727651
8 2.776365   0.009189 -1.742022
8 1.473293 -1.657397   2.206163
8 0.697490   2.716910   1.148407
1 -1.611143   1.585134 -1.282362
1 -2.509150 -1.373565   0.930956
1 -4.282110   0.273954   1.135168
1 -0.558738   0.601694 -2.418127
1 -3.638614   1.209892 -0.330805
6 -0.649816 -1.678137 -0.910128
1 -0.887550 -2.562311 -0.321499
1 -0.087417 -1.868425 -1.821041

xyz coordinates of structure 22

6 -2.490363 -0.430135   0.305567
6 -1.556515 -0.772181 -0.779069
6 -0.560546 -1.771990 -0.680170
6 0.092955 -2.069879   0.546892
26 0.356261 -0.026033   0.022918
6 -0.074307   1.673271 -0.388372
6 1.826779 -0.122285 -1.090275
6 1.204568   0.289701   1.587919
8 -0.358859   2.765784 -0.647916
8 2.755454 -0.193268 -1.778055
8 1.756556   0.473465   2.590001
1 -2.329710 -0.902078   1.275917
1 -1.864019 -0.465342 -1.778574
1 -0.122961 -2.143603 -1.605667
1 0.926391 -2.767980   0.533947
1 -0.454713 -2.039969   1.487425
6 -3.550825   0.394407   0.160399
1 -3.764815   0.890372 -0.786200
1 -4.228631   0.592154   0.987707

xyz coordinates of structure 22ts

6 -1.813124 -0.678643   0.028972
6 -1.150097 -1.040280 -1.192513
6 0.064430 -1.772607 -1.102087
6 0.555127 -2.098718   0.204287
26 0.229919 -0.013382 -0.007789
6 -0.212456   1.617633 -0.629437
6 1.963890   0.251324 -0.403869
6 0.225091   0.259565   1.759047
8 -0.499358   2.673168 -1.008732
8 3.088419   0.398128 -0.637876
8 0.210236   0.409375   2.907709
1 -1.836878 -1.443212   0.811296
1 -1.481754 -0.644046 -2.150781
1 0.661421 -1.936944 -1.997107
1 1.566292 -2.495505   0.275890
1 -0.121671 -2.484503   0.963717
6 -3.001055   0.208565   0.013919
1 -3.972682 -0.191284 -0.279890
1 -2.977851   1.217036   0.420661

xyz coordinates of structure 22'

6 -2.544287   0.393370   0.206496
6 -1.595597 -0.184605 -0.812722
6 -0.974079 -1.450174 -0.659028
6 -0.504634 -1.893212   0.600851
26 0.386894 -0.027189   0.043925
6 0.392122   1.751348 -0.239145
6 1.708974 -0.441101 -1.196773
6 1.417816 -0.065870   1.523106
8 0.392702   2.895523 -0.424782
8 2.533034 -0.704630 -1.965408
8 2.072284 -0.101677   2.478698
1 -1.760577   0.148184 -1.838253
1 -0.621273 -1.959545 -1.555827
1 0.078520 -2.809126   0.658087
1 -1.054960 -1.630730   1.503803
6 -3.851573   0.090157   0.235634
1 -2.166638   1.114783   0.933504
1 -4.518357   0.545579   0.966309
1 -4.292566 -0.615438 -0.468259

xyz coordinates of structure 23

6 -2.508312   0.578314 -0.258505
6 -1.502655 -0.042745 -1.151388
6 -0.938835 -1.338704 -1.024913
6 -0.631462 -1.937335   0.222398
26 0.324983 -0.029158   0.022254
6 0.427325   1.767862 -0.040793
6 1.815518 -0.355418 -1.037570
6 1.092868 -0.259861   1.638204
8 0.493194   2.924541 -0.081910
8 2.743781 -0.565191 -1.696403
8 1.582962 -0.423299   2.675284
1 -1.445460   0.406596 -2.143650
1 -0.473188 -1.762913 -1.914251
1 -0.051468 -2.857324   0.224335
1 -1.265802 -1.789104   1.091109

1 -2.571830   1.665583 -0.338096
6 -3.372266 -0.044526   0.569616
1 -4.088286   0.528565   1.155084
1 -3.406120 -1.127218   0.668805

xyz coordinates of structure 24

6 1.018330 -1.504500 -.384187
6 1.514564 -.308796 -.952015
6 2.724143 .401991 -.492568
6 3.678124 -.073980 .330929
26 -.499138 -.049148 -.153297
6 -2.280708 -.248422 -.317897
6 -.423218   1.736967 -.396245
6 -.409944 -.035242   1.704573
8 -3.425951 -.389928 -.425470
8 -.370407   2.883894 -.555451
8 -.358283 -.024751   2.860125
1 1.451195 -1.858324   .551191
1 1.214256 -.089085 -1.981422
1 2.841525   1.412609 -.888564
1 4.529199   .542136   .612681
1 3.647939 -1.083001   .739406
6 -.210912 -2.055040 -.815043
1 -.500609 -1.973453 -1.863790
1 -.631073 -2.904643 -.282693