

Supporting Information For:

Assessment of Stereoelectronic Factors that Influence the CO₂ Fixation

Ability of N-Heterocyclic Carbenes: A DFT Study

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Table S1. Values of $\Delta V_{\min 1}$ and $\Delta V_{\min 2}$ in kcal/mol.

Systems	$\Delta V_{\min 1}$	$\Delta V_{\min 2}$
ImNH ₂	0.0	0.0
ImMe ₂	-4.0	-3.8
ImEt ₂	-4.1	-4.0
Im ⁱ Pr ₂	-4.4	-4.8
Im(OMe) ₂	-0.7	-2.4
Im(NMe ₂) ₂	-4.4	-6.3
ImPh ₂	1.6	-3.6
ImF ₂	12.0	7.9
ImCl ₂	12.7	5.8
Im(CF ₃) ₂	20.5	11.2
Im(CN) ₂	28.4	16.2
Im(NO ₂) ₂	30.7	18.1
Im(CO ₂ Me) ₂	10.3	3.6
ImNMe ₂	-1.6	-3.5
ImNEt ₂	-1.9	-2.0
ImN ⁱ Pr ₂	-2.8	-1.8
ImNcy ₂	-3.6	-3.2
ImN(OMe) ₂	13.5	2.4
ImN(NMe ₂) ₂	7.5	3.8
ImNPh ₂	7.7	0.3
ImNMes ₂	-0.8	-2.6
ImN(CO ₂ Me) ₂	25.8	13.6
ImNMe ₂	15.5	4.4
ImNEt ₂	23.8	10.2
ImN ⁱ Pr ₂	34.5	16.3
ImNcy ₂	10.5	7.9

$\Delta V_{\min 1}$ is the difference in $V_{\min 1}$ between corresponding NHC and ImNH₂ and $\Delta V_{\min 2}$ is the difference in $V_{\min 2}$ between corresponding NHC-CO₂ and ImNH₂-CO₂.

Table S2. Values of V_{pred1} and V_{pred2} in kcal/mol.

Systems	V_{pred1}	V_{pred2}
Im(NO ₂) ₂ NMe ₂	-54.1	-67.6
Im(CF ₃) ₂ NMe ₂	-64.3	-74.6
ImNMe ₂ N(Me) ₂	-89.2	-92.1
ImCl ₂ NMe ₂	-72.0	-79.9
Im(CN) ₂ NMe ₂	-56.4	-69.6
Im(CO ₂ Me) ₂ NMe ₂	-74.5	-82.2
ImF ₂ NMe ₂	-72.7	-77.9
ImMe ₂ NMe ₂	-88.8	-89.5
ImMe ₂ N(OMe) ₂	-73.7	-83.6
ImMe ₂ N(NMe ₂) ₂	-79.6	-82.2
ImEt ₂ N(OMe) ₂	-73.7	-83.9
ImEt ₂ N(NMe ₂) ₂	-79.7	-82.5
ImPh ₂ N(OMe) ₂	-68.1	-83.4
ImPh ₂ N(NMe ₂) ₂	-74.0	-82.0
ImCl ₂ N ⁱ Pr ₂	-73.2	-78.2
Im(NO ₂) ₂ N ⁱ Pr ₂	-55.3	-65.9
ImF ₂ NPh ₂	-63.4	-74.1

V_{pred1} and V_{pred2} are the predicted V_{min1} and V_{min2} respectively using additivity of the substituents.

Table S3. Cartesian coordinates of all the geometries (in Å), SCF energy (in a.u) and number of imaginary frequencies (N_{img}).

System Coordinates			
<u>ImNH₂</u>			
At. No.	x	y	z
6	-0.000001000	-1.262597000	-0.000048000
7	1.039905000	-0.398959000	0.000133000
7	-1.039906000	-0.398957000	-0.000151000
6	0.672146000	0.927302000	0.000121000
6	-0.672145000	0.927303000	-0.000065000
1	1.986012000	-0.721760000	0.000258000
1	-1.986012000	-0.721758000	-0.000287000
1	-1.373078000	1.738446000	-0.000137000
1	1.373081000	1.738444000	0.000243000
E = -226.081471956		N _{img} =0	
<u>ImMe₂</u>			
At. No.	x	y	z
6	-0.000001000	1.937962000	-0.000108000
7	1.037252000	1.073481000	-0.000025000
7	-1.037253000	1.073480000	-0.000103000
6	0.674436000	-0.261189000	0.000037000
6	-0.674436000	-0.261190000	-0.000016000
1	1.984561000	1.394283000	-0.000023000
1	-1.984563000	1.394281000	-0.000151000
6	1.661493000	-1.362992000	-0.000026000
1	2.301541000	-1.326927000	-0.880339000
1	2.303008000	-1.325644000	0.879159000
1	1.158689000	-2.324867000	0.001128000
6	-1.661492000	-1.362994000	0.000191000
1	-2.301392000	-1.326951000	0.880613000
1	-2.303153000	-1.325625000	-0.878886000
1	-1.158686000	-2.324868000	-0.001072000
E = -304.679485108		N _{img} =0	
<u>ImEt₂</u>			
At. No.	x	y	z
6	0.000017000	2.263913000	-0.000016000
7	0.987163000	1.399339000	-0.319066000
7	-0.987147000	1.399368000	0.319055000
6	0.641827000	0.064464000	-0.209305000
6	-0.641840000	0.064483000	0.209327000
1	1.887242000	1.722129000	-0.612287000
1	-1.887218000	1.722185000	0.612273000

6	1.588064000	-1.039429000	-0.502667000
1	1.919309000	-0.970260000	-1.540231000
1	1.052546000	-1.982702000	-0.420260000
6	-1.588102000	-1.039384000	0.502708000
1	-1.052585000	-1.982666000	0.420401000
1	-1.919409000	-0.970139000	1.540247000
6	-2.800035000	-1.055325000	-0.417044000
1	-3.368633000	-0.130771000	-0.342169000
1	-2.497264000	-1.170277000	-1.454536000
1	-3.468645000	-1.873980000	-0.162566000
6	2.800053000	-1.055311000	0.417012000
1	3.368654000	-0.130767000	0.342032000
1	2.497346000	-1.170184000	1.454531000
1	3.468642000	-1.873989000	0.162553000
E = -383.263523894 N _{img} =0			

ImⁱPr₂

At. No.	x	y	z
6	0.000001000	2.445012000	-0.000344000
7	1.037295000	1.580657000	0.000074000
7	-1.037294000	1.580657000	-0.000137000
6	0.674850000	0.244799000	0.000048000
6	-0.674849000	0.244799000	-0.000052000
1	1.983494000	1.904951000	0.000223000
1	-1.983493000	1.904950000	-0.000209000
6	1.673558000	-0.859408000	0.000100000
1	1.111677000	-1.793265000	0.000483000
6	-1.673557000	-0.859408000	0.000073000
1	-1.111677000	-1.793265000	0.000008000
6	-2.537847000	-0.827123000	1.254106000
1	-1.930818000	-0.881405000	2.153783000
1	-3.120639000	0.091925000	1.302859000
1	-3.238308000	-1.659476000	1.259554000
6	2.538309000	-0.826822000	1.253802000
1	3.121229000	0.092173000	1.302066000
1	1.931614000	-0.880772000	2.153725000
1	3.238691000	-1.659239000	1.259241000
6	-2.538164000	-0.827150000	-1.253737000
1	-3.120939000	0.091915000	-1.302394000
1	-1.931375000	-0.881504000	-2.153571000
1	-3.238662000	-1.659472000	-1.258964000
6	2.537700000	-0.827453000	-1.254042000
1	1.930574000	-0.882158000	-2.153628000
1	3.120331000	0.091674000	-1.303201000
1	3.238291000	-1.659699000	-1.259273000
E = -461.849897907 N _{img} =0			

Im(OMe)₂

At. No.	x	y	z
6	-2.422648000	0.023707000	-0.000449000
7	-1.545278000	0.997701000	-0.331387000
7	-1.576370000	-0.982178000	0.322855000
6	-0.224846000	0.624316000	-0.218670000
6	-0.246755000	-0.656897000	0.196427000
1	-1.834363000	1.900733000	-0.651084000
1	-1.893739000	-1.877997000	0.635907000
8	0.786005000	1.454459000	-0.516915000
6	1.610247000	1.783477000	0.585558000
1	1.027644000	2.258809000	1.372031000
1	2.095762000	0.894679000	0.985687000
1	2.359793000	2.473040000	0.215256000
8	0.727739000	-1.527369000	0.494331000
6	1.662141000	-1.736885000	-0.547032000
1	1.164221000	-2.122674000	-1.434273000
1	2.179046000	-0.813073000	-0.800070000
1	2.374382000	-2.465213000	-0.178055000
E = -455.016494737		N _{img} =0	

Im(NMe₂)₂

At. No.	x	y	z
6	-0.001694000	2.544300000	-0.000089000
7	1.037116000	1.682931000	-0.063178000
7	-1.039794000	1.681752000	0.063148000
6	0.674637000	0.346474000	-0.037489000
6	-0.676061000	0.345849000	0.036880000
1	1.980659000	2.007226000	-0.125775000
1	-1.983655000	2.005232000	0.125017000
7	1.556928000	-0.727427000	-0.076351000
7	-1.557380000	-0.728629000	0.077848000
6	-1.505840000	-1.580117000	-1.090096000
1	-1.938130000	-1.100491000	-1.975272000
1	-0.472440000	-1.836568000	-1.303742000
1	-2.055010000	-2.496856000	-0.888548000
6	-2.893116000	-0.415442000	0.504746000
1	-2.865986000	0.134798000	1.441801000
1	-3.458768000	0.169220000	-0.233586000
1	-3.438190000	-1.339702000	0.675972000
6	1.513592000	-1.570597000	1.097987000
1	1.950413000	-1.084157000	1.977211000
1	0.481870000	-1.827100000	1.319620000
1	2.062853000	-2.488035000	0.899796000

6	2.889787000	-0.415204000	-0.512997000
1	2.856228000	0.130414000	-1.452520000
1	3.459324000	0.173774000	0.218904000
1	3.434912000	-1.339724000	-0.682795000
E = -493.875237703		N _{img} =0	

ImPh₂

At. No.	x	y	z
6	0.000015000	3.415439000	-0.000035000
7	-1.037466000	2.552120000	0.013203000
7	1.037490000	2.552110000	-0.013208000
6	-0.678555000	1.218102000	0.014577000
6	0.678567000	1.218095000	-0.014516000
1	-1.985251000	2.866455000	0.080699000
1	1.985277000	2.866433000	-0.080730000
6	-1.655561000	0.138167000	0.080983000
6	-1.421421000	-0.979767000	0.877417000
6	-2.849806000	0.216697000	-0.630522000
6	-2.351561000	-1.998382000	0.948074000
6	-3.784363000	-0.800851000	-0.550435000
6	-3.537509000	-1.912800000	0.235893000
1	-0.507234000	-1.040263000	1.447453000
1	-3.036510000	1.068294000	-1.268785000
1	-2.155605000	-2.857841000	1.570575000
1	-4.703149000	-0.727315000	-1.111724000
1	-4.265422000	-2.706992000	0.295378000
6	1.655564000	0.138154000	-0.080956000
6	1.421377000	-0.979791000	-0.877360000
6	2.849840000	0.216684000	0.630499000
6	2.351506000	-1.998414000	-0.948045000
6	3.784392000	-0.800867000	0.550372000
6	3.537494000	-1.912824000	-0.235930000
1	0.507147000	-1.040303000	-1.447323000
1	3.036582000	1.068293000	1.268732000
1	2.155511000	-2.857886000	-1.570514000
1	4.703207000	-0.727326000	1.111613000
1	4.265399000	-2.707021000	-0.295439000
E = -687.998690888		N _{img} =0	

ImF₂

At. No.	x	y	z
6	0.000007000	1.849228000	-0.000325000
7	-1.046566000	0.988545000	0.000203000
7	1.046573000	0.988537000	-0.000098000
6	-0.667608000	-0.325901000	0.000075000
6	0.667605000	-0.325906000	-0.000097000

1	-1.999178000	1.295997000	0.000427000
1	1.999189000	1.295981000	-0.000147000
9	-1.536365000	-1.311998000	0.000258000
9	1.536355000	-1.312010000	-0.000139000
E = -424.487105653		N _{img} =0	

ImCl₂

At. No.	x	y	z
6	0.000000000	2.311409000	0.000317000
7	1.043868000	1.452434000	-0.000188000
7	-1.043868000	1.452434000	0.000139000
6	0.672223000	0.130934000	-0.000042000
6	-0.672223000	0.130934000	0.000109000
1	1.995881000	1.761984000	-0.000417000
1	-1.995881000	1.761984000	0.000207000
17	-1.767847000	-1.155815000	0.000155000
17	1.767847000	-1.155815000	-0.000258000
E = -1145.36746091		N _{img} =0	

Im(CF₃)₂

At. No.	x	y	z
6	0.000000000	2.746031000	0.000000000
7	-1.040468000	1.883599000	0.017009000
7	1.040468000	1.883599000	-0.017008000
6	-0.673144000	0.563679000	0.012765000
6	0.673144000	0.563679000	-0.012766000
1	-1.993288000	2.192524000	0.050194000
1	1.993288000	2.192524000	-0.050193000
6	1.669181000	-0.535877000	0.000564000
9	1.275178000	-1.572486000	-0.723403000
9	2.825695000	-0.093613000	-0.498942000
9	1.920582000	-0.976415000	1.229996000
6	-1.669181000	-0.535877000	-0.000564000
9	-1.275178000	-1.572486000	0.723403000
9	-2.825695000	-0.093613000	0.498942000
9	-1.920582000	-0.976415000	-1.229996000
E = -899.999837870		N _{img} =0	

Im(CN)₂

At. No.	x	y	z
6	-0.000002000	2.265415000	-0.000533000
7	-1.042567000	1.407435000	0.000444000
7	1.042565000	1.407436000	-0.000249000
6	-0.678827000	0.082944000	-0.000092000
6	0.678827000	0.082944000	-0.000067000
1	-1.994427000	1.720917000	0.000908000

1	1.994425000	1.720920000	-0.000374000
6	-1.591168000	-0.991888000	0.000081000
7	-2.363881000	-1.845081000	0.000247000
6	1.591169000	-0.991886000	-0.000016000
7	2.363884000	-1.845078000	0.000019000
E = -410.478806312		N _{img} =0	

Im(NO₂)₂

At. No.	x	y	z
6	0.000007000	2.473757000	0.000004000
7	1.043122000	1.609744000	-0.004738000
7	-1.043114000	1.609750000	0.004737000
6	0.677502000	0.301830000	0.000139000
6	-0.677503000	0.301834000	-0.000154000
1	2.007527000	1.891400000	-0.015365000
1	-2.007517000	1.891414000	0.015366000
7	-1.675664000	-0.718537000	-0.050783000
8	-2.801844000	-0.337263000	0.190224000
8	-1.342949000	-1.832997000	-0.347448000
7	1.675657000	-0.718548000	0.050756000
8	2.801846000	-0.337268000	-0.190197000
8	1.342942000	-1.832998000	0.347454000
E = -634.899079385		N _{img} =0	

Im(CO₂Me)₂

At. No.	x	y	z
6	0.000006000	2.704600000	0.000034000
7	1.037544000	1.839732000	0.000042000
7	-1.037536000	1.839735000	-0.000010000
6	0.680582000	0.515908000	0.000055000
6	-0.680579000	0.515910000	-0.000030000
1	1.995585000	2.132946000	0.000077000
1	-1.995576000	2.132952000	-0.000062000
6	-1.688579000	-0.548840000	-0.000256000
8	-1.487301000	-1.727107000	-0.000811000
8	-2.910370000	-0.004526000	0.000319000
6	-3.981205000	-0.934537000	0.000113000
1	-3.933821000	-1.561186000	-0.884506000
1	-3.932070000	-1.563613000	0.882896000
1	-4.886517000	-0.342150000	0.001759000
6	1.688577000	-0.548844000	0.000235000
8	1.487294000	-1.727110000	0.000943000
8	2.910367000	-0.004530000	-0.000422000
6	3.981203000	-0.934541000	-0.000192000
1	3.934116000	-1.560815000	0.884712000
1	3.931767000	-1.563992000	-0.882689000

1 4.886514000 -0.342154000 -0.002380000
 E = -681.656674466 N_{img}=0

ImNMe₂

At. No.	x	y	z
6	0.000000000	-0.970588000	0.000009000
7	1.052160000	-0.120161000	-0.000001000
7	-1.052160000	-0.120161000	0.000009000
6	0.672642000	1.200966000	-0.000039000
6	-0.672642000	1.200966000	-0.000021000
6	2.418818000	-0.565842000	-0.000003000
6	-2.418818000	-0.565842000	0.000038000
1	-2.940874000	-0.211944000	-0.885620000
1	-2.940834000	-0.211953000	0.885722000
1	-2.408167000	-1.648367000	0.000032000
1	2.408167000	-1.648367000	0.000076000
1	2.940875000	-0.211883000	0.885629000
1	2.940833000	-0.212013000	-0.885712000
1	1.372588000	2.014407000	-0.000061000
1	-1.372588000	2.014407000	-0.000025000

E = -304.655564478 N_{img}=0

ImNEt₂

At. No.	x	y	z
6	0.000004000	-0.885546000	0.000023000
7	-1.011366000	-0.036407000	-0.291616000
6	0.647302000	1.285061000	0.183548000
7	1.011371000	-0.036390000	0.291628000
6	-0.647309000	1.285051000	-0.183570000
6	2.342117000	-0.485350000	0.624747000
6	3.318530000	-0.292697000	-0.514289000
6	-2.342106000	-0.485387000	-0.624734000
6	-3.318540000	-0.292671000	0.514273000
1	-3.409011000	0.756654000	0.786451000
1	-2.987620000	-0.843345000	1.390611000
1	-4.305098000	-0.652696000	0.232291000
1	4.305097000	-0.652694000	-0.232303000
1	3.408984000	0.756612000	-0.786534000
1	2.987599000	-0.843428000	-1.390586000
1	-2.677254000	0.045438000	-1.514656000
1	-2.248184000	-1.535891000	-0.877775000
1	2.248202000	-1.535840000	0.877849000
1	2.677280000	0.045526000	1.514632000
1	1.321005000	2.099251000	0.371201000

1 -1.321018000 2.099230000 -0.371248000
E = -383.246660609 N_{img}=0

ImNⁱPr₂

At. No.	x	y	z
6	0.000000000	-0.000021000	0.937692000
7	1.053638000	-0.000005000	0.089878000
7	-1.053638000	-0.000004000	0.089878000
6	0.672746000	-0.000039000	-1.231400000
6	-0.672746000	-0.000038000	-1.231400000
6	2.430596000	0.000020000	0.547739000
6	-2.430596000	0.000022000	0.547739000
6	3.147104000	1.257365000	0.097953000
6	3.147120000	-1.257341000	0.098024000
6	-3.147118000	-1.257342000	0.098030000
6	-3.147106000	1.257363000	0.097948000
1	1.367900000	-0.000047000	-2.049116000
1	-1.367900000	-0.000044000	-2.049116000
1	2.347489000	0.000050000	1.630990000
1	2.615416000	-2.143413000	0.433436000
1	4.154940000	-1.283321000	0.505154000
1	3.226464000	-1.296419000	-0.987456000
1	2.615385000	2.143450000	0.433310000
1	4.154921000	1.283385000	0.505086000
1	3.226454000	1.296382000	-0.987529000
1	-2.347489000	0.000056000	1.630990000
1	-3.226457000	1.296375000	-0.987534000
1	-2.615388000	2.143450000	0.433300000
1	-4.154923000	1.283383000	0.505082000
1	-3.226460000	-1.296426000	-0.987451000
1	-4.154938000	-1.283322000	0.505158000
1	-2.615412000	-2.143413000	0.433446000

E = -461.838107291 N_{img}=0

ImNcy₂

At. No.	x	y	z
6	0.000000000	-0.011441000	-0.753437000
7	1.054352000	-0.129766000	0.085896000
7	-1.054352000	-0.129766000	0.085896000
6	0.672856000	-0.305363000	1.395467000
6	-0.672856000	-0.305363000	1.395467000
6	2.425043000	-0.015808000	-0.365008000
6	3.083051000	1.238030000	0.184529000
6	4.501568000	1.377306000	-0.336047000
6	5.327124000	0.144760000	-0.013714000
6	4.662103000	-1.109629000	-0.551753000

6	3.243591000	-1.249459000	-0.027953000
6	-2.425043000	-0.015808000	-0.365008000
6	-3.083051000	1.238030000	0.184529000
6	-4.501568000	1.377306000	-0.336047000
6	-5.327124000	0.144761000	-0.013714000
6	-4.662104000	-1.109629000	-0.551752000
6	-3.243591000	-1.249460000	-0.027952000
1	1.367251000	-0.418100000	2.205908000
1	-1.367251000	-0.418100000	2.205908000
1	2.346412000	0.072512000	-1.447418000
1	2.480538000	2.104672000	-0.081783000
1	3.099064000	1.182572000	1.276087000
1	4.473412000	1.518565000	-1.418697000
1	4.966722000	2.269068000	0.081042000
1	6.332821000	0.244271000	-0.419511000
1	5.433721000	0.057393000	1.070202000
1	4.637691000	-1.063689000	-1.642668000
1	5.243965000	-1.992392000	-0.291450000
1	2.757960000	-2.131113000	-0.442589000
1	3.271983000	-1.380102000	1.056775000
1	-2.346412000	0.072512000	-1.447417000
1	-2.480537000	2.104672000	-0.081784000
1	-3.099063000	1.182572000	1.276086000
1	-4.473411000	1.518565000	-1.418698000
1	-4.966722000	2.269068000	0.081041000
1	-5.433721000	0.057394000	1.070202000
1	-6.332821000	0.244272000	-0.419511000
1	-4.637691000	-1.063690000	-1.642667000
1	-5.243966000	-1.992392000	-0.291449000
1	-3.271983000	-1.380102000	1.056776000
1	-2.757960000	-2.131113000	-0.442588000
E = -695.212638754		N _{img} =0	

ImN(OMe)₂

At. No.	x	y	z
6	-0.000002000	-0.699739000	-0.000002000
7	0.991759000	0.167417000	0.240620000
7	-0.991761000	0.167422000	-0.240618000
6	0.656524000	1.492433000	0.156161000
6	-0.656519000	1.492436000	-0.156157000
1	-1.358197000	2.282878000	-0.331061000
1	1.358204000	2.282872000	0.331067000
8	-2.246624000	-0.206627000	-0.602638000
6	-2.887721000	-0.904185000	0.447523000
1	-2.326746000	-1.798615000	0.701819000
1	-2.994156000	-0.264872000	1.322382000

1	-3.863341000	-1.168573000	0.056960000
8	2.246620000	-0.206639000	0.602641000
6	2.887723000	-0.904178000	-0.447529000
1	2.326747000	-1.798601000	-0.701848000
1	2.994166000	-0.264847000	-1.322374000
1	3.863339000	-1.168578000	-0.056965000
E = -454.908782665		N _{img} =0	

ImN(NMe₂)₂

At. No.	x	y	z
6	0.000000000	-0.469184000	0.000200000
7	1.037920000	0.388383000	-0.000003000
7	-1.037920000	0.388383000	-0.000039000
6	0.672588000	1.714540000	-0.000182000
6	-0.672588000	1.714540000	-0.000178000
1	-1.396626000	2.504556000	-0.000312000
1	1.396626000	2.504557000	-0.000301000
7	-2.380750000	0.015473000	-0.000064000
7	2.380750000	0.015473000	0.000004000
6	-2.696905000	-0.729175000	1.200428000
1	-3.766622000	-0.918674000	1.211403000
1	-2.158564000	-1.678742000	1.250628000
1	-2.442152000	-0.130969000	2.069634000
6	-2.696762000	-0.729621000	-1.200317000
1	-3.766477000	-0.919129000	-1.211349000
1	-2.441909000	-0.131735000	-2.069713000
1	-2.158411000	-1.679203000	-1.250102000
6	2.696853000	-0.729305000	1.200429000
1	3.766581000	-0.918737000	1.211468000
1	2.441988000	-0.131221000	2.069686000
1	2.158565000	-1.678910000	1.250474000
6	2.696814000	-0.729491000	-1.200315000
1	2.442063000	-0.131487000	-2.069661000
1	3.766520000	-0.919059000	-1.211288000
1	2.158416000	-1.679039000	-1.250250000
E = -493.817708922		N _{img} =0	

ImNPh₂

At. No.	x	y	z
6	0.000000000	0.364023000	-0.063927000
7	-1.054083000	-0.455992000	0.169346000
7	1.054084000	-0.455991000	0.169346000
6	-0.670035000	-1.730509000	0.537595000
6	0.670036000	-1.730506000	0.537602000
1	1.365109000	-2.500453000	0.806946000
1	-1.365108000	-2.500457000	0.806936000

6	-2.397890000	-0.049692000	0.022654000
6	-2.741998000	1.277390000	0.226690000
6	-3.367666000	-0.975377000	-0.326582000
6	-4.059769000	1.668313000	0.086023000
6	-4.686318000	-0.575804000	-0.453529000
6	-5.038764000	0.745976000	-0.247670000
1	-1.967628000	1.980743000	0.484363000
1	-3.093662000	-1.999849000	-0.523839000
1	-4.323994000	2.702249000	0.246004000
1	-5.436293000	-1.301445000	-0.727776000
1	-6.066599000	1.056842000	-0.350435000
6	2.397890000	-0.049692000	0.022654000
6	3.367666000	-0.975376000	-0.326587000
6	2.741998000	1.277389000	0.226694000
6	4.686317000	-0.575804000	-0.453534000
6	4.059770000	1.668312000	0.086027000
6	5.038764000	0.745976000	-0.247669000
1	3.093660000	-1.999848000	-0.523847000
1	1.967629000	1.980741000	0.484370000
1	5.436292000	-1.301444000	-0.727784000
1	4.323996000	2.702248000	0.246012000
1	6.066598000	1.056842000	-0.350435000
E = -687.975546812 N _{img} =0			

ImNMes₂

At. No.	x	y	z
6	0.000050000	0.000751000	-0.275192000
7	-1.051595000	-0.011850000	0.580083000
7	1.051587000	0.012077000	0.580392000
6	-0.671661000	-0.008378000	1.906958000
6	0.671359000	0.006355000	1.907085000
1	1.379130000	0.015794000	2.713392000
1	-1.379636000	-0.018966000	2.713060000
6	-2.407667000	-0.024687000	0.154206000
6	-3.143866000	1.151068000	0.209158000
6	-2.959450000	-1.217253000	-0.303324000
6	-4.471044000	1.110985000	-0.195952000
6	-4.286002000	-1.210179000	-0.700454000
6	-5.058718000	-0.057475000	-0.651943000
1	-5.054601000	2.020415000	-0.161286000
1	-4.728149000	-2.129933000	-1.058298000
6	2.407645000	0.024898000	0.154452000
6	3.143769000	-1.150911000	0.209080000
6	2.959521000	1.217463000	-0.302906000
6	4.470922000	-1.110898000	-0.196117000
6	4.286072000	1.210336000	-0.700154000

6	5.058711000	0.057600000	-0.651934000
1	5.054359000	-2.020411000	-0.161645000
1	4.728198000	2.130164000	-1.057841000
6	2.514209000	-2.426518000	0.669003000
1	1.605640000	-2.632401000	0.106664000
1	3.197026000	-3.260518000	0.539265000
1	2.233293000	-2.381699000	1.719669000
6	2.133639000	2.460267000	-0.376154000
1	2.747817000	3.315539000	-0.641288000
1	1.346324000	2.350219000	-1.118859000
1	1.645797000	2.666692000	0.574588000
6	6.488721000	0.082526000	-1.092252000
1	6.958113000	-0.888380000	-0.963001000
1	6.570262000	0.355269000	-2.142630000
1	7.063058000	0.810510000	-0.522855000
6	-2.133323000	-2.459874000	-0.376756000
1	-2.747615000	-3.315739000	-0.639709000
1	-1.347384000	-2.350390000	-1.121020000
1	-1.643580000	-2.664889000	0.573316000
6	-2.514209000	2.426482000	0.669540000
1	-1.606094000	2.633133000	0.106743000
1	-3.197303000	3.260471000	0.541135000
1	-2.232413000	2.380554000	1.719920000
6	-6.488775000	-0.082495000	-1.092115000
1	-6.958455000	0.888171000	-0.962112000
1	-6.570328000	-0.354480000	-2.142696000
1	-7.062820000	-0.811083000	-0.523214000
E = -923.748571984 N _{img} =0			

ImN(CO₂Me)₂

At. No.	x	y	z
6	0.000000000	-0.389045000	0.000015000
7	1.044281000	0.481067000	-0.000697000
7	-1.044281000	0.481067000	0.000705000
6	0.665999000	1.822591000	-0.000614000
6	-0.665999000	1.822591000	0.000613000
1	-1.388367000	2.613533000	0.001397000
1	1.388367000	2.613532000	-0.001408000
6	-2.397234000	0.122826000	0.001568000
8	-3.267042000	0.948829000	0.005617000
8	-2.569233000	-1.173911000	-0.003288000
6	-3.924725000	-1.593690000	-0.003138000
1	-4.427120000	-1.242207000	0.892056000
1	-4.438319000	-1.206967000	-0.877102000
1	-3.890572000	-2.674402000	-0.024168000

6	2.397234000	0.122826000	-0.001564000
8	3.267042000	0.948828000	-0.005626000
8	2.569232000	-1.173912000	0.003290000
6	3.924726000	-1.593689000	0.003129000
1	4.427134000	-1.242138000	-0.892031000
1	4.438304000	-1.207029000	0.877131000
1	3.890574000	-2.674402000	0.024081000
E = -681.648823991		N _{img} =0	

Im(NO₂)₂NMe₂

At. No.	x	y	z
6	0.000013000	2.139367000	-0.000005000
7	-1.064872000	1.299072000	-0.015986000
7	1.064886000	1.299059000	0.015982000
6	-0.676707000	-0.004466000	-0.010686000
6	0.676703000	-0.004476000	0.010666000
7	1.581397000	-1.106738000	0.081717000
8	2.659142000	-0.949721000	-0.447084000
8	1.211689000	-2.086124000	0.676143000
7	-1.581421000	-1.106712000	-0.081746000
8	-2.659121000	-0.949720000	0.447153000
8	-1.211730000	-2.086104000	-0.676171000
6	2.425121000	1.794852000	0.079107000
1	2.959873000	1.547823000	-0.829482000
1	2.344879000	2.867117000	0.197139000
1	2.947804000	1.364827000	0.926714000
6	-2.425102000	1.794881000	-0.079102000
1	-2.959852000	1.547857000	0.829490000
1	-2.344849000	2.867146000	-0.197134000
1	-2.947794000	1.364863000	-0.926707000
E = -713.472954841		N _{img} =0	

Im(CF₃)₂NMe₂

At. No.	x	y	z
7	-1.054768000	1.518659000	-0.000044000
7	1.054768000	1.518659000	-0.000002000
6	0.000000000	2.361475000	-0.000032000
6	-2.412556000	2.020963000	-0.000086000
6	-0.678251000	0.195670000	-0.000025000
6	0.678251000	0.195670000	0.000008000
6	2.412556000	2.020963000	0.000026000
1	-2.333281000	3.099801000	-0.000087000
1	2.333279000	3.099801000	0.000006000
1	-2.946473000	1.695143000	-0.886089000
1	-2.946530000	1.695158000	0.885888000

1	2.946476000	1.695164000	0.886034000
1	2.946527000	1.695139000	-0.885942000
6	1.721295000	-0.867722000	0.000000000
6	-1.721295000	-0.867722000	0.000023000
9	1.243294000	-2.094559000	0.000083000
9	2.511479000	-0.747133000	-1.071539000
9	2.511594000	-0.747041000	1.071445000
9	-1.243294000	-2.094559000	-0.000082000
9	-2.511435000	-0.747135000	1.071596000
9	-2.511637000	-0.747040000	-1.071389000
E = -978.570775255		N _{img} =0	

ImNMe₂N(Me)₂

At. No.	x	y	z
7	1.186269000	1.374661000	-0.084851000
7	-0.916155000	1.437421000	0.033162000
6	0.158055000	2.251061000	-0.000115000
6	2.559683000	1.786571000	-0.175297000
6	0.772562000	0.058225000	-0.106742000
6	-0.579292000	0.087356000	-0.021293000
6	-2.259668000	1.945521000	0.060807000
1	2.570933000	2.822464000	-0.490167000
1	-2.746899000	1.829673000	-0.905137000
1	3.066021000	1.706891000	0.785099000
1	3.081231000	1.166038000	-0.897670000
1	-2.851573000	1.435111000	0.816112000
1	-2.199786000	2.999917000	0.301180000
6	-2.430076000	-1.112847000	-1.020166000
1	-3.322257000	-0.491991000	-0.878933000
1	-1.969023000	-0.842127000	-1.965325000
1	-2.758369000	-2.149469000	-1.086026000
6	2.368641000	-1.337434000	0.987955000
1	1.721015000	-1.889879000	1.678591000
1	3.229850000	-1.959261000	0.753164000
1	2.723945000	-0.445527000	1.494669000
7	1.686356000	-0.979796000	-0.234465000
7	-1.465918000	-0.982421000	0.043037000
6	1.237422000	-2.132928000	-0.975961000
1	2.106028000	-2.725184000	-1.258246000
1	0.550992000	-2.766404000	-0.408719000
1	0.732915000	-1.808888000	-1.880882000
6	-1.991598000	-1.311109000	1.344837000
1	-2.813319000	-0.657263000	1.661467000
1	-2.369572000	-2.332659000	1.333675000
1	-1.200374000	-1.247001000	2.084808000
E = -572.449821236		N _{img} =0	

ImCl₂NMe₂

At. No.	x	y	z
7	1.058593000	1.083762000	-0.000053000
7	-1.058593000	1.083762000	0.000033000
6	0.000000000	1.927315000	-0.000130000
6	2.425931000	1.532869000	-0.000037000
6	0.673046000	-0.232843000	-0.000065000
6	-0.673046000	-0.232843000	-0.000012000
6	-2.425931000	1.532869000	0.000179000
1	2.398893000	2.614734000	-0.000017000
1	-2.398893000	2.614734000	0.000120000
1	2.947444000	1.179542000	0.884980000
1	2.947437000	1.179576000	-0.885071000
1	-2.947540000	1.179513000	-0.884768000
1	-2.947340000	1.179605000	0.885283000
17	-1.752158000	-1.537781000	0.000071000
17	1.752158000	-1.537781000	-0.000071000
E = -1223.94455977		N _{img} =0	

Im(CN)₂NMe₂

At. No.	x	y	z
7	1.056329000	1.004839000	-0.000095000
7	-1.056329000	1.004839000	0.000101000
6	0.000000000	1.848608000	-0.000090000
6	2.429958000	1.448719000	-0.000160000
6	0.679995000	-0.314270000	-0.000085000
6	-0.679995000	-0.314270000	0.000004000
6	-2.429958000	1.448719000	0.000315000
1	2.413353000	2.530178000	-0.000101000
1	-2.413353000	2.530178000	0.000256000
1	2.944696000	1.088291000	0.885253000
1	2.944567000	1.088387000	-0.885686000
1	-2.944775000	1.088292000	-0.885051000
1	-2.944488000	1.088386000	0.885888000
6	-1.588712000	-1.392442000	0.000074000
6	1.588712000	-1.392442000	-0.000128000
7	-2.359188000	-2.248370000	-0.000013000
7	2.359187000	-2.248371000	-0.000013000
E = -489.057852821		N _{img} =0	

Im(CO₂Me)₂NMe₂

At. No.	x	y	z
8	1.194962000	-1.674397000	0.905746000
8	2.600588000	-0.514684000	-0.377935000
8	-2.905132000	-0.569457000	0.504384000

8	-1.295441000	-1.780527000	-0.452063000
7	0.907277000	1.756637000	-0.017397000
7	-1.207107000	1.747401000	-0.060576000
6	-0.154452000	2.593843000	-0.094661000
6	2.257257000	2.267719000	0.026851000
6	0.533754000	0.437730000	0.067289000
6	1.444039000	-0.699616000	0.252525000
6	3.545266000	-1.560529000	-0.218604000
6	-2.569547000	2.221861000	-0.148651000
6	-0.825741000	0.434354000	0.033857000
6	-1.786649000	-0.672615000	0.070717000
6	-2.127259000	-2.923233000	-0.348710000
1	-1.560299000	-3.737233000	-0.779942000
1	4.421493000	-1.253036000	-0.773935000
1	-2.355623000	-3.126600000	0.692500000
1	-3.052929000	-2.767213000	-0.893618000
1	3.783340000	-1.698007000	0.831379000
1	3.147108000	-2.489077000	-0.614522000
1	2.776802000	1.903498000	0.907925000
1	2.174769000	3.345745000	0.070717000
1	2.811504000	1.970131000	-0.856048000
1	-3.118464000	1.971382000	0.751306000
1	-3.075782000	1.772876000	-0.997496000
1	-2.512935000	3.294698000	-0.277194000
E = -760.227507013 N _{img} =0			

ImF₂NMe₂

At. No.	x	y	z
7	1.059205000	-0.641080000	-0.000036000
7	-1.059205000	-0.641080000	-0.000040000
6	0.000000000	-1.487586000	-0.000496000
6	2.432789000	-1.070630000	0.000247000
6	0.668202000	0.667610000	-0.000111000
6	-0.668202000	0.667610000	-0.000114000
6	-2.432789000	-1.070630000	0.000228000
1	2.420029000	-2.152995000	0.000125000
1	-2.420029000	-2.152995000	0.000135000
1	2.949328000	-0.710289000	-0.884672000
1	2.948980000	-0.710484000	0.885452000
1	-2.948996000	-0.710459000	0.885413000
1	-2.949312000	-0.710314000	-0.884711000
9	-1.534052000	1.660245000	0.000011000
9	1.534052000	1.660245000	0.000019000
E = -503.064890520 N _{img} =0			

ImMe₂NMe₂

At. No.	x	y	z
7	-1.049418000	0.703081000	0.000018000
7	1.049418000	0.703081000	0.000058000
6	0.000000000	1.553655000	-0.000092000
6	-2.413215000	1.151961000	0.000113000
6	-0.675095000	-0.628575000	-0.000103000
6	0.675095000	-0.628575000	-0.000071000
6	2.413215000	1.151961000	0.000237000
1	-2.396861000	2.234494000	0.000191000
1	2.396861000	2.234494000	0.000216000
1	-2.941734000	0.802185000	-0.884372000
1	-2.941682000	0.802055000	0.884577000
1	2.941602000	0.802136000	0.884782000
1	2.941814000	0.802104000	-0.884167000
6	1.651621000	-1.740232000	-0.000082000
1	2.295411000	-1.712476000	0.878258000
1	1.135959000	-2.695539000	-0.000333000
1	2.295713000	-1.712178000	-0.878190000
6	-1.651621000	-1.740232000	-0.000161000
1	-2.295458000	-1.712471000	0.878145000
1	-2.295666000	-1.712183000	-0.878303000
1	-1.135959000	-2.695539000	-0.000379000
E = -383.253318890		N _{img} =0	

ImMe₂N(OMe)₂

At. No.	x	y	z
6	0.000000000	-1.229525000	-0.000002000
7	-0.997020000	-0.361611000	-0.202413000
7	0.997019000	-0.361611000	0.202412000
6	-0.664186000	0.974496000	-0.132066000
6	0.664186000	0.974496000	0.132065000
8	2.265405000	-0.736768000	0.518448000
6	2.877577000	-1.401908000	-0.567823000
1	2.309456000	-2.289104000	-0.832426000
1	2.958345000	-0.739187000	-1.428490000
1	3.864855000	-1.677066000	-0.215031000
8	-2.265406000	-0.736768000	-0.518447000
6	-2.877576000	-1.401909000	0.567824000
1	-2.309454000	-2.289105000	0.832426000
1	-2.958342000	-0.739188000	1.428492000
1	-3.864854000	-1.677066000	0.215034000
6	1.646462000	2.058543000	0.338553000
1	2.102564000	1.992611000	1.323413000
1	2.447864000	2.015296000	-0.396000000
1	1.159968000	3.024657000	0.250538000

6	-1.646462000	2.058543000	-0.338552000
1	-2.102565000	1.992611000	-1.323412000
1	-2.447864000	2.015296000	0.396001000
1	-1.159969000	3.024657000	-0.250537000
E = -533.508804420		N _{img} =0	

ImMe₂N(NMe₂)₂

At. No.	x	y	z
6	0.000000000	-0.941713000	-0.000464000
7	-1.035648000	-0.085048000	-0.000182000
7	1.035647000	-0.085048000	-0.000017000
6	-0.674803000	1.253175000	-0.000205000
6	0.674803000	1.253175000	0.000101000
7	2.375793000	-0.463600000	0.000153000
7	-2.375793000	-0.463600000	-0.000008000
6	2.692102000	-1.207660000	-1.200072000
1	3.760979000	-1.403346000	-1.210249000
1	2.148037000	-2.153939000	-1.253418000
1	2.441200000	-0.608045000	-2.069751000
6	2.691646000	-1.208493000	1.199979000
1	3.760448000	-1.404596000	1.210170000
1	2.440878000	-0.609303000	2.069989000
1	2.147229000	-2.154599000	1.252659000
6	-2.691972000	-1.208209000	-1.199919000
1	-3.760777000	-1.404300000	-1.209850000
1	-2.441446000	-0.608817000	-2.069860000
1	-2.147576000	-2.154307000	-1.252972000
6	-2.691777000	-1.207944000	1.200132000
1	-2.440632000	-0.608532000	2.069881000
1	-3.760650000	-1.403641000	1.210570000
1	-2.147691000	-2.154230000	1.253105000
6	1.669006000	2.346372000	0.000346000
1	2.312343000	2.296252000	0.875824000
1	2.315150000	2.293871000	-0.872909000
1	1.167114000	3.309011000	-0.001735000
6	-1.669006000	2.346373000	-0.000066000
1	-2.312498000	2.296397000	-0.875437000
1	-2.314995000	2.293728000	0.873296000
1	-1.167113000	3.309011000	0.002092000
E = -572.416445396		N _{img} =0	

ImEt₂N(OMe)₂

At. No.	x	y	z
6	-0.000121000	-1.582833000	-0.000021000
7	-1.017520000	-0.715141000	-0.003217000
7	1.017403000	-0.715285000	0.003148000

6	-0.677320000	0.622325000	-0.007604000
6	0.677383000	0.622231000	0.007549000
8	2.323712000	-1.094212000	-0.028403000
6	2.686429000	-1.746309000	1.172199000
1	2.577544000	-1.073892000	2.022163000
1	2.075523000	-2.632635000	1.316924000
1	3.727117000	-2.021655000	1.045128000
8	-2.323896000	-1.093857000	0.028389000
6	-2.686581000	-1.746589000	-1.171878000
1	-2.577648000	-1.074634000	-2.022200000
1	-2.075697000	-2.633010000	-1.316098000
1	-3.727280000	-2.021833000	-1.044684000
6	1.682591000	1.710521000	-0.025146000
1	1.182139000	2.644794000	0.220408000
1	2.419922000	1.538707000	0.758617000
6	2.389319000	1.827412000	-1.367335000
1	1.678902000	2.047947000	-2.160247000
1	2.893204000	0.896712000	-1.612697000
1	3.131040000	2.622342000	-1.344148000
6	-1.682360000	1.710773000	0.025035000
1	-1.181748000	2.644956000	-0.220535000
1	-2.419697000	1.539052000	-0.758741000
6	-2.389098000	1.827842000	1.367204000
1	-1.678662000	2.048293000	2.160123000
1	-2.893150000	0.897243000	1.612600000
1	-3.130681000	2.622900000	1.343964000
E = -612.094216447 N _{img} =0			

ImEt₂N(NMe₂)₂

At. No.	x	y	z
6	0.000047000	1.290440000	-0.000030000
7	-1.029648000	0.435006000	0.119884000
7	1.029703000	0.434979000	-0.119990000
6	-0.670539000	-0.903633000	0.080327000
6	0.670545000	-0.903658000	-0.080528000
7	2.355537000	0.821834000	-0.306087000
7	-2.355458000	0.821918000	0.306097000
6	2.799649000	1.651038000	0.793699000
1	3.858678000	1.855901000	0.661474000
1	2.249297000	2.593213000	0.847563000
1	2.662651000	1.111460000	1.726160000
6	2.509821000	1.487025000	-1.582547000
1	3.565374000	1.694073000	-1.736997000
1	2.166751000	0.827206000	-2.373759000
1	1.944349000	2.421163000	-1.629693000
6	-2.509639000	1.486948000	1.582660000

1	-3.565180000	1.693952000	1.737263000
1	-2.166469000	0.827039000	2.373755000
1	-1.944184000	2.421095000	1.629878000
6	-2.799576000	1.651293000	-0.793558000
1	-2.662929000	1.111715000	-1.726074000
1	-3.858518000	1.856432000	-0.661083000
1	-2.248975000	2.593316000	-0.847478000
6	1.650892000	-2.011101000	-0.176987000
1	1.105974000	-2.929663000	-0.386638000
1	2.307088000	-1.833564000	-1.027753000
6	2.493081000	-2.180877000	1.077879000
1	1.865327000	-2.377568000	1.943880000
1	3.068705000	-1.279692000	1.270464000
1	3.190253000	-3.008623000	0.967929000
6	-1.650896000	-2.011078000	0.176831000
1	-1.105920000	-2.929677000	0.386139000
1	-2.306830000	-1.833690000	1.027843000
6	-2.493483000	-2.180618000	-1.077804000
1	-1.866005000	-2.376888000	-1.944101000
1	-3.069354000	-1.279484000	-1.269864000
1	-3.190432000	-3.008555000	-0.967887000
E =	-651.001704266	N _{img} =0	

ImPh₂N(OMe)₂

At. No.	x	y	z
6	-0.001418000	2.775230000	0.000025000
7	1.015024000	1.911725000	-0.105985000
7	-1.017027000	1.910706000	0.105759000
6	0.678150000	0.572687000	-0.059376000
6	-0.678855000	0.572039000	0.059195000
8	-2.304412000	2.315985000	0.237727000
6	-2.854541000	2.653734000	-1.021026000
1	-2.279626000	3.455746000	-1.476440000
1	-2.878656000	1.782185000	-1.673330000
1	-3.864315000	2.987345000	-0.812152000
8	2.301966000	2.318524000	-0.237377000
6	2.853182000	2.650253000	1.022494000
1	2.278401000	3.449809000	1.482413000
1	2.878259000	1.775489000	1.670451000
1	3.862642000	2.985274000	0.814365000
6	-1.634751000	-0.531535000	0.055743000
6	-1.445305000	-1.588272000	-0.831736000
6	-2.726956000	-0.562002000	0.918445000
6	-2.320185000	-2.656954000	-0.849496000
6	-3.604493000	-1.631779000	0.892466000
6	-3.404347000	-2.682001000	0.012486000

1	-0.606188000	-1.565634000	-1.510206000
1	-2.882474000	0.253008000	1.606738000
1	-2.159310000	-3.468246000	-1.542585000
1	-4.445991000	-1.645339000	1.568067000
1	-4.090919000	-3.514391000	-0.002483000
6	1.635071000	-0.529985000	-0.056083000
6	1.446200000	-1.587319000	0.830821000
6	2.727803000	-0.559002000	-0.918198000
6	2.322053000	-2.655196000	0.848516000
6	3.606359000	-1.627951000	-0.892207000
6	3.406718000	-2.678808000	-0.012878000
1	0.606830000	-1.565754000	1.509003000
1	2.882900000	0.256445000	-1.606070000
1	2.161575000	-3.466961000	1.541142000
1	4.448257000	-1.640358000	-1.567335000
1	4.094080000	-3.510545000	0.002065000
E = -916.825114308 N _{img} =0			

ImPh₂N(NMe₂)₂

At. No.	x	y	z
6	-0.000319000	-2.413754000	-0.000432000
7	-1.040118000	-1.563294000	0.008783000
7	1.039724000	-1.563594000	-0.009827000
6	-0.679127000	-0.223963000	0.001690000
6	0.679147000	-0.224200000	-0.001856000
7	2.370582000	-1.967509000	0.050632000
7	-2.371075000	-1.966884000	-0.051024000
6	2.675662000	-2.876818000	-1.030935000
1	3.739251000	-3.096546000	-0.998366000
1	2.107608000	-3.807587000	-0.964931000
1	2.448539000	-2.396449000	-1.978617000
6	2.666934000	-2.530639000	1.349438000
1	3.729509000	-2.752935000	1.392114000
1	2.438587000	-1.797055000	2.116493000
1	2.095361000	-3.442628000	1.542471000
6	-2.667651000	-2.532657000	-1.348634000
1	-3.730356000	-2.754430000	-1.390876000
1	-2.438811000	-1.800875000	-2.117248000
1	-2.096592000	-3.445380000	-1.539643000
6	-2.676575000	-2.873796000	1.032451000
1	-2.448917000	-2.391672000	1.979112000
1	-3.740323000	-3.092877000	1.000562000
1	-2.109149000	-3.805076000	0.968193000
6	1.621323000	0.891589000	0.050931000
6	1.399260000	1.938532000	0.940716000
6	2.733956000	0.944368000	-0.783264000

6	2.265122000	3.015199000	0.992270000
6	3.600450000	2.020516000	-0.728114000
6	3.369762000	3.059396000	0.158648000
1	0.542193000	1.902047000	1.595802000
1	2.916930000	0.136181000	-1.472588000
1	2.078614000	3.818105000	1.688857000
1	4.458591000	2.048628000	-1.382125000
1	4.048253000	3.897608000	0.200196000
6	-1.621041000	0.892020000	-0.051185000
6	-1.398671000	1.938948000	-0.940894000
6	-2.733679000	0.945050000	0.782980000
6	-2.264281000	3.015831000	-0.992439000
6	-3.599941000	2.021387000	0.727824000
6	-3.368962000	3.060253000	-0.158888000
1	-0.541526000	1.902369000	-1.595872000
1	-2.916873000	0.136885000	1.472280000
1	-2.077490000	3.818770000	-1.688911000
1	-4.458135000	2.049673000	1.381758000
1	-4.047263000	3.898620000	-0.200452000
E = -955.730497631 N _{img} =0			

ImCl₂NNⁱPr₂

At. No.	x	y	z
6	-0.000022000	-1.583881000	-0.000097000
7	-1.066615000	-0.750526000	-0.000157000
7	1.066589000	-0.750555000	0.000097000
6	-0.674008000	0.564317000	-0.000099000
6	0.674016000	0.564285000	0.000010000
6	-2.425757000	-1.282030000	0.000043000
6	2.425718000	-1.282064000	-0.000059000
6	-3.174684000	-0.915531000	-1.265315000
6	-3.174162000	-0.915586000	1.265731000
6	3.174522000	-0.915589000	1.265377000
6	3.174205000	-0.915553000	-1.265673000
17	-1.695956000	1.920732000	-0.000164000
17	1.696052000	1.920619000	0.000193000
1	-2.249562000	-2.354040000	0.000009000
1	-2.599476000	-1.197128000	2.143928000
1	-4.120692000	-1.449849000	1.292497000
1	-3.390915000	0.147545000	1.318375000
1	-2.600218000	-1.196652000	-2.143791000
1	-4.121022000	-1.450158000	-1.291897000
1	-3.391853000	0.147525000	-1.317618000
1	2.249534000	-2.354078000	-0.000083000
1	3.391054000	0.147563000	-1.318228000
1	2.599545000	-1.196980000	-2.143923000

1	4.120686000	-1.449901000	-1.292420000
1	3.391357000	0.147528000	1.317912000
1	4.121025000	-1.449927000	1.291877000
1	2.600122000	-1.197056000	2.143784000
E = -1381.12256091		N _{img} =0	

Im(NO₂)₂NⁱPr₂

At. No.	x	y	z
6	0.001744000	-1.753668000	-0.003037000
7	-1.071534000	-0.925320000	-0.023894000
7	1.073666000	-0.923982000	0.020051000
6	-0.676271000	0.377102000	-0.010201000
6	0.676410000	0.378249000	0.009776000
6	-2.422390000	-1.503147000	-0.128404000
6	2.425013000	-1.500837000	0.125061000
6	-3.227274000	-0.883206000	-1.251109000
6	-3.132020000	-1.511296000	1.208928000
6	3.225762000	-0.886374000	1.253708000
6	3.139183000	-1.501460000	-1.209874000
1	-2.190893000	-2.529600000	-0.397175000
1	-2.518025000	-2.004005000	1.957791000
1	-4.059974000	-2.069582000	1.112487000
1	-3.366440000	-0.507985000	1.545779000
1	-2.653137000	-0.853981000	-2.173934000
1	-4.105982000	-1.497712000	-1.426841000
1	-3.575550000	0.116819000	-1.012964000
1	2.193538000	-2.528912000	0.387584000
1	3.376427000	-0.496478000	-1.539682000
1	2.527280000	-1.988771000	-1.963974000
1	4.065945000	-2.061748000	-1.113480000
1	3.573273000	0.115485000	1.022332000
1	4.104786000	-1.500716000	1.428511000
1	2.648796000	-0.863294000	2.174943000
7	1.525106000	1.529485000	0.049974000
8	1.165540000	2.440998000	0.751740000
8	2.533615000	1.496570000	-0.616005000
7	-1.528284000	1.526442000	-0.048075000
8	-1.177862000	2.435307000	-0.757628000
8	-2.530498000	1.493615000	0.627285000
E = -870.649615093		N _{img} =0	

ImF₂NPh₂

At. No.	x	y	z
6	0.000000000	-0.649339000	0.127258000
7	-1.064348000	0.180846000	-0.028041000
7	1.064349000	0.180847000	-0.028041000

6	-0.666938000	1.472593000	-0.272411000
6	0.666938000	1.472593000	-0.272413000
9	1.503431000	2.458667000	-0.507694000
9	-1.503433000	2.458667000	-0.507688000
6	-2.407117000	-0.261662000	0.056993000
6	-2.720152000	-1.526800000	-0.410785000
6	-3.382781000	0.547135000	0.614669000
6	-4.021495000	-1.981570000	-0.318710000
6	-4.685659000	0.085743000	0.687840000
6	-5.009825000	-1.176485000	0.223667000
1	-1.936381000	-2.137825000	-0.826999000
1	-3.130584000	1.522561000	0.996515000
1	-4.264585000	-2.968570000	-0.680306000
1	-5.446291000	0.716738000	1.120432000
1	-6.026173000	-1.532552000	0.286508000
6	2.407118000	-0.261661000	0.056993000
6	3.382782000	0.547136000	0.614670000
6	2.720152000	-1.526799000	-0.410784000
6	4.685660000	0.085743000	0.687840000
6	4.021495000	-1.981570000	-0.318709000
6	5.009825000	-1.176485000	0.223668000
1	3.130585000	1.522562000	0.996516000
1	1.936380000	-2.137824000	-0.826999000
1	5.446292000	0.716737000	1.120432000
1	4.264585000	-2.968570000	-0.680306000
1	6.026173000	-1.532553000	0.286509000
E = -886.378508456 N _{img} =0			

ImBicar

At. No.	x	y	z
6	-0.000034000	-1.656787000	-0.000147000
7	-1.028301000	-0.783586000	-0.050317000
7	1.028301000	-0.783602000	0.049442000
6	-0.671783000	0.552590000	-0.034504000
6	0.671782000	0.552559000	0.033477000
6	-1.886002000	1.402695000	-0.124491000
6	-2.986773000	0.399631000	0.256465000
6	-2.453396000	-0.963369000	-0.182136000
6	1.885903000	1.402722000	0.124383000
6	2.987033000	0.399585000	-0.255402000
6	2.453277000	-0.963392000	0.182663000
1	1.866518000	2.264582000	-0.536583000
1	2.028755000	1.771936000	1.140807000
1	3.113965000	0.402266000	-1.335886000
1	3.946489000	0.634826000	0.195064000
1	2.797156000	-1.784488000	-0.436807000

1	2.707499000	-1.182576000	1.219417000
1	-2.029934000	1.771569000	-1.140901000
1	-1.865913000	2.264784000	0.536143000
1	-3.946639000	0.634880000	-0.193143000
1	-3.112720000	0.402258000	1.337056000
1	-2.708707000	-1.182624000	-1.218600000
1	-2.796502000	-1.784503000	0.437711000
E = -459.437061743		N _{img} =0	

ImCylm

At. No.	x	y	z
7	1.048038000	-0.890956000	-0.018426000
7	-1.048032000	-0.890958000	-0.018520000
6	0.000002000	-1.741317000	-0.044153000
6	2.421482000	-1.326618000	-0.128468000
6	3.365526000	-0.249612000	0.359189000
6	3.046497000	1.074901000	-0.310322000
6	1.663957000	1.544258000	0.110452000
6	0.674970000	0.439841000	0.001606000
6	-0.674970000	0.439843000	0.001540000
6	-1.663957000	1.544266000	0.110390000
6	-3.046559000	1.074898000	-0.310178000
6	-3.365482000	-0.249671000	0.359273000
6	-2.421475000	-1.326592000	-0.128635000
1	-1.712230000	1.892565000	1.145130000
1	-1.341049000	2.396121000	-0.486456000
1	-3.082807000	0.948239000	-1.393399000
1	-3.787772000	1.828077000	-0.051877000
1	-4.387838000	-0.556988000	0.149709000
1	-3.276869000	-0.141446000	1.441623000
1	-2.522681000	-2.247759000	0.435684000
1	-2.636574000	-1.554673000	-1.173258000
1	1.712375000	1.892455000	1.145221000
1	1.340964000	2.396167000	-0.486269000
1	3.787748000	1.828098000	-0.052186000
1	3.082563000	0.948171000	-1.393540000
1	3.277076000	-0.141277000	1.441542000
1	4.387856000	-0.556941000	0.149513000
1	2.522711000	-2.247651000	0.436067000
1	2.636543000	-1.554951000	-1.173040000
E = -538.040643504		N _{img} =0	

ImPhen

At. No.	x	y	z
7	1.061106000	-1.295250000	-0.119848000
7	-1.061110000	-1.295249000	-0.119850000

6	-0.000003000	-2.146965000	-0.113749000
6	2.475064000	-1.583412000	-0.138222000
6	3.228701000	-0.435460000	0.531281000
6	2.923136000	0.947341000	-0.058926000
6	1.440975000	1.168720000	-0.085083000
6	0.683024000	0.021251000	-0.124511000
6	-0.683024000	0.021251000	-0.124507000
6	-1.440972000	1.168721000	-0.085070000
6	-2.923134000	0.947347000	-0.058924000
6	-3.228704000	-0.435455000	0.531280000
6	-2.475069000	-1.583406000	-0.138227000
1	-3.326344000	1.011931000	-1.071274000
1	-3.425516000	1.715204000	0.525895000
1	-4.295227000	-0.637763000	0.463435000
1	-2.970586000	-0.427320000	1.590076000
1	-2.647311000	-2.520518000	0.381114000
1	-2.807139000	-1.704218000	-1.169903000
1	3.425517000	1.715198000	0.525894000
1	3.326351000	1.011924000	-1.071275000
1	2.970583000	-0.427321000	1.590077000
1	4.295223000	-0.637772000	0.463437000
1	2.647302000	-2.520521000	0.381126000
1	2.807134000	-1.704232000	-1.169897000
6	-0.703048000	2.344297000	-0.047459000
6	0.703058000	2.344302000	-0.047464000
1	-1.216451000	3.293852000	-0.001685000
1	1.216469000	3.293850000	-0.001645000
E = -613.033500741 N _{img} =0			

IMPhenPh₂

At. No.	x	y	z
7	1.103081000	0.316442000	-0.210540000
7	-0.794860000	-0.118023000	0.639011000
6	0.371145000	-0.722173000	0.281546000
6	2.419172000	0.314937000	-0.825978000
6	3.027477000	1.715717000	-0.648258000
6	2.162876000	2.869462000	-1.162885000
6	0.789554000	2.770493000	-0.574536000
6	0.418655000	1.506834000	-0.177099000
6	-0.799297000	1.227024000	0.375898000
6	-1.766232000	2.177502000	0.610394000
6	-3.013153000	1.658552000	1.257557000
6	-2.683167000	0.389273000	2.049712000
6	-1.978917000	-0.703364000	1.222685000
1	-3.761631000	1.428902000	0.496833000
1	-3.453291000	2.400755000	1.920210000

1	-3.593780000	-0.035222000	2.465286000
1	-2.032427000	0.651367000	2.883882000
1	-1.655816000	-1.497480000	1.891394000
1	2.634205000	3.817186000	-0.910093000
1	2.104632000	2.831750000	-2.252299000
1	3.218127000	1.860469000	0.415517000
1	3.994224000	1.720235000	-1.145566000
1	2.290758000	0.125116000	-1.893353000
6	-1.413831000	3.464732000	0.226381000
6	-0.168175000	3.752765000	-0.355116000
1	-2.108972000	4.276633000	0.383619000
1	0.048647000	4.775495000	-0.627751000
6	3.329015000	-0.741347000	-0.268181000
6	3.500203000	-0.891207000	1.101538000
6	4.060869000	-1.543327000	-1.127511000
6	4.389404000	-1.824993000	1.598190000
6	4.955877000	-2.478899000	-0.633444000
6	5.122161000	-2.621261000	0.731771000
1	2.915527000	-0.288978000	1.781032000
1	3.923554000	-1.443492000	-2.194925000
1	4.506317000	-1.938367000	2.665150000
1	5.514633000	-3.100442000	-1.316266000
1	5.812841000	-3.353292000	1.121388000
6	-2.913841000	-1.289327000	0.193843000
6	-2.917156000	-0.874070000	-1.128857000
6	-3.839220000	-2.241509000	0.599951000
6	-3.834213000	-1.397554000	-2.026345000
6	-4.753842000	-2.767372000	-0.294029000
6	-4.754968000	-2.343721000	-1.612999000
1	-2.193202000	-0.145894000	-1.462945000
1	-3.836077000	-2.582163000	1.626373000
1	-3.823288000	-1.066667000	-3.053705000
1	-5.460377000	-3.513471000	0.036258000
1	-5.464523000	-2.754385000	-2.314716000
E = -1074.93437044 N _{img} =0			

ImDpylm

At. No.	x	y	z
7	-1.045275000	0.852662000	-0.000011000
7	1.045277000	0.852661000	-0.000008000
6	0.000000000	1.720725000	-0.000066000
6	-2.369199000	1.217227000	0.000020000
6	-3.329688000	0.274522000	0.000036000
6	-2.990471000	-1.111451000	0.000021000
6	-1.688638000	-1.486536000	-0.000012000
6	-0.686749000	-0.496010000	-0.000028000

6	0.686748000	-0.496010000	-0.000037000
6	1.688637000	-1.486536000	-0.000019000
6	2.990470000	-1.111450000	0.000018000
6	3.329689000	0.274522000	0.000039000
6	2.369199000	1.217225000	0.000025000
1	1.399822000	-2.525502000	-0.000027000
1	3.773031000	-1.852460000	0.000037000
1	4.361977000	0.581995000	0.000055000
1	2.544004000	2.278650000	0.000018000
1	-1.399821000	-2.525502000	-0.000024000
1	-3.773034000	-1.852458000	0.000034000
1	-4.361976000	0.581994000	0.000051000
1	-2.544002000	2.278651000	0.000016000

E = -533.194754614 N_{img}=0

BImNMe₂

At. No.	x	y	z
7	-1.162098000	-1.064445000	-0.000047000
7	-1.162098000	1.064445000	-0.000121000
6	-1.999406000	0.000000000	-0.000278000
6	-1.613714000	-2.426585000	0.000220000
6	0.165515000	-0.695066000	0.000017000
6	0.165515000	0.695066000	-0.000063000
6	-1.613710000	2.426588000	-0.000223000
1	-2.696145000	-2.413291000	-0.001034000
1	-2.696142000	2.413295000	0.000398000
1	-1.257761000	-2.950468000	-0.884470000
1	-1.259828000	-2.949563000	0.886281000
1	-1.258276000	2.950234000	0.884817000
1	-1.259304000	2.949799000	-0.885935000
6	1.344161000	1.417868000	-0.000036000
1	1.347082000	2.496678000	-0.000106000
6	1.344158000	-1.417870000	0.000161000
1	1.347079000	-2.496681000	0.000266000
6	2.526094000	0.696715000	0.000094000
6	2.526094000	-0.696718000	0.000193000
1	3.467213000	1.223944000	0.000133000
1	3.467213000	-1.223948000	0.000311000

E = -458.245924104 N_{img}=0

BImNEt₂

At. No.	x	y	z
7	0.864114000	-0.399542000	1.065043000
7	0.864114000	-0.399542000	-1.065043000
6	1.690718000	-0.522679000	0.000000000
6	1.320897000	-0.435800000	2.432269000

6	-0.449539000	-0.200339000	0.694958000
6	-0.449539000	-0.200339000	-0.694958000
6	1.320897000	-0.435800000	-2.432269000
1	2.303266000	-0.895070000	2.411576000
1	2.303266000	-0.895070000	-2.411576000
1	0.658009000	-1.088847000	2.999509000
1	0.658009000	-1.088847000	-2.999509000
6	-1.618985000	-0.042764000	-1.416898000
1	-1.621844000	-0.045225000	-2.495966000
6	-1.618985000	-0.042764000	1.416898000
1	-1.621844000	-0.045225000	2.495966000
6	-2.790088000	0.117380000	-0.696924000
6	-2.790088000	0.117380000	0.696924000
1	-3.722348000	0.244933000	-1.224481000
1	-3.722348000	0.244933000	1.224481000
6	1.381492000	0.941369000	3.056565000
1	0.406788000	1.423487000	3.045503000
1	1.715122000	0.874808000	4.089294000
1	2.077397000	1.571675000	2.509743000
6	1.381492000	0.941369000	-3.056565000
1	1.715122000	0.874808000	-4.089294000
1	0.406788000	1.423487000	-3.045503000
1	2.077397000	1.571675000	-2.509743000
E = -536.836447693 N _{img} =0			

Py[b]ImNMe₂

At. No.	x	y	z
7	1.037789000	1.143627000	-0.000020000
7	1.229942000	-0.985132000	-0.000109000
6	1.965938000	0.156446000	-0.000104000
6	1.352209000	2.546888000	0.000169000
6	-0.243694000	0.652704000	0.000041000
6	-0.120056000	-0.736046000	-0.000036000
6	1.812376000	-2.297394000	-0.000308000
1	2.430690000	2.637682000	-0.000953000
1	2.888085000	-2.175215000	0.000188000
1	0.937982000	3.027953000	-0.881147000
1	0.939909000	3.027354000	0.882724000
1	1.512666000	-2.853486000	0.885423000
1	1.513426000	-2.852920000	-0.886654000
6	-1.261277000	-1.506857000	-0.000025000
1	-1.233729000	-2.585474000	-0.000099000
7	-1.365410000	1.333471000	0.000154000
6	-2.460209000	-0.807487000	0.000087000
6	-2.462728000	0.583193000	0.000172000
1	-3.399549000	-1.336068000	0.000109000

1 -3.401075000 1.117727000 0.000261000
E = -474.283101881 N_{img}=0

Py[c]ImNMe₂

At. No.	x	y	z
7	-1.156079000	-1.057490000	-0.000056000
7	-1.142927000	1.075914000	-0.000006000
6	-1.986279000	0.008603000	0.000114000
6	-1.612220000	-2.419953000	0.000052000
6	0.171636000	-0.687579000	0.000051000
6	0.176320000	0.700498000	0.000048000
6	-1.594963000	2.439617000	-0.000317000
1	-2.694469000	-2.402682000	-0.001944000
1	-2.677295000	2.424578000	0.000953000
1	-1.257163000	-2.943567000	-0.884561000
1	-1.260466000	-2.942410000	0.886672000
1	-1.240379000	2.962612000	0.884859000
1	-1.242468000	2.961669000	-0.886892000
6	1.376262000	1.385514000	0.000015000
1	1.438385000	2.461704000	-0.000060000
6	1.367194000	-1.379223000	0.000098000
1	1.405451000	-2.459411000	0.000147000
6	2.515549000	0.597895000	0.000047000
7	2.521826000	-0.733194000	0.000088000
1	3.487664000	1.068664000	-0.000001000

E = -474.276798443 N_{img}=0

CO₂

At. No.	x	y	z
6	0.000000000	0.000000000	0.000408000
8	0.000000000	1.155301000	-0.000153000
8	0.000000000	-1.155301000	-0.000153000

E = -188.509223665 N_{img}=0

ImNH₂-CO₂

At. No.	x	y	z
6	-0.031099000	-0.000024000	-0.000019000
7	0.754598000	-1.060330000	0.000084000
7	0.754561000	1.060308000	0.000016000
6	2.068273000	-0.676303000	-0.000196000
6	2.068249000	0.676331000	0.000131000
1	0.349096000	-1.982668000	0.000143000
1	0.348994000	1.982620000	0.000056000
1	2.881186000	1.374208000	0.000235000
1	2.881234000	-1.374153000	-0.000344000
6	-1.563018000	-0.000004000	-0.000020000

8	-2.017470000	-1.141780000	0.000069000
8	-2.017411000	1.141799000	-0.000090000
E =	-414.616842747	N _{img} =0	

ImMe₂-CO₂

At. No.	x	y	z
6	-0.754108000	-0.000291000	-0.000042000
7	0.032173000	-1.057945000	0.000129000
7	0.031796000	1.057666000	-0.000025000
6	1.355830000	-0.679748000	0.000167000
6	1.355508000	0.679885000	0.000049000
1	-0.372482000	-1.980319000	0.000193000
1	-0.373394000	1.979811000	-0.000098000
6	2.464173000	-1.658569000	0.000360000
1	2.428727000	-2.295664000	0.881238000
1	2.428364000	-2.296395000	-0.879970000
1	3.418909000	-1.144649000	-0.000063000
6	2.463706000	1.658864000	-0.000027000
1	2.428332000	2.295899000	-0.880949000
1	2.427675000	2.296749000	0.880250000
1	3.418473000	1.145002000	0.000591000
6	-2.282371000	-0.000095000	-0.000151000
8	-2.742135000	-1.140924000	-0.000081000
8	-2.741467000	1.141079000	-0.000427000
E =	-493.218843929	N _{img} =0	

ImEt₂-CO₂

At. No.	x	y	z
6	1.195845000	-0.000009000	-0.000020000
7	0.410265000	1.015561000	0.296708000
7	0.410264000	-1.015577000	-0.296750000
6	-0.914050000	0.652651000	0.192668000
6	-0.914046000	-0.652665000	-0.192706000
1	0.817908000	1.898544000	0.558799000
1	0.817905000	-1.898562000	-0.558837000
6	-2.022467000	1.601976000	0.457506000
1	-1.952224000	1.957255000	1.485739000
1	-2.959334000	1.055343000	0.389318000
6	-2.022479000	-1.601970000	-0.457542000
1	-2.959327000	-1.055289000	-0.389473000
1	-1.952172000	-1.957340000	-1.485739000
6	-2.040547000	-2.785293000	0.498405000
1	-1.123946000	-3.367084000	0.433563000
1	-2.150285000	-2.453768000	1.527356000
1	-2.867211000	-3.450014000	0.264283000
6	-2.040415000	2.785380000	-0.498342000

1	-1.123812000	3.367152000	-0.433357000
1	-2.150055000	2.453940000	-1.527330000
1	-2.867083000	3.450104000	-0.264240000
6	2.723269000	-0.000023000	0.000009000
8	3.183458000	1.095078000	0.320353000
8	3.183451000	-1.095135000	-0.320310000
E = -571.803733532		N _{img} =0	

ImⁱPr₂-CO₂

At. No.	x	y	z
6	-1.486224000	-0.000315000	-0.000196000
7	-0.701064000	1.057706000	-0.000066000
7	-0.700593000	-1.058029000	-0.000050000
6	0.624429000	0.680290000	0.000041000
6	0.624762000	-0.680105000	0.000122000
1	-1.110307000	1.977975000	-0.000095000
1	-1.109247000	-1.978538000	-0.000067000
6	1.731159000	1.676300000	0.000094000
1	2.659581000	1.107362000	0.000333000
6	1.731791000	-1.675824000	0.000318000
1	2.660102000	-1.106710000	0.000368000
6	1.698041000	-2.535826000	1.256967000
1	1.748254000	-1.928866000	2.156797000
1	0.785235000	-3.127803000	1.303546000
1	2.536059000	-3.228184000	1.263004000
6	1.697116000	2.536543000	1.256564000
1	0.784233000	3.128420000	1.302929000
1	1.747327000	1.929780000	2.156530000
1	2.535045000	3.229006000	1.262528000
6	1.698299000	-2.536022000	-1.256202000
1	0.785508000	-3.128016000	-1.302868000
1	1.748686000	-1.929204000	-2.156118000
1	2.536324000	-3.228372000	-1.261961000
6	1.697548000	2.536207000	-1.256621000
1	1.748098000	1.929200000	-2.156403000
1	0.784662000	3.128040000	-1.303472000
1	2.535460000	3.228690000	-1.262473000
6	-3.012909000	-0.000398000	-0.000391000
8	-3.474265000	-1.141152000	-0.000602000
8	-3.474172000	1.140449000	-0.000141000
E = -650.390764666		N _{img} =0	

Im(OMe)₂-CO₂

At. No.	x	y	z
6	-1.317142000	-0.008659000	-0.005840000
7	-0.528900000	1.011924000	-0.285211000

7	-0.538608000	-1.041095000	0.265418000
6	0.787398000	0.634398000	-0.187096000
6	0.779275000	-0.681412000	0.154937000
1	-0.916334000	1.906496000	-0.542072000
1	-0.933308000	-1.933624000	0.518053000
8	1.788147000	1.473718000	-0.439753000
6	2.607130000	1.778575000	0.682319000
1	2.017362000	2.242970000	1.468482000
1	3.083798000	0.878142000	1.064341000
1	3.359352000	2.471113000	0.326905000
8	1.759170000	-1.541896000	0.408750000
6	2.726051000	-1.678137000	-0.624312000
1	2.252458000	-2.017880000	-1.541801000
1	3.236662000	-0.734936000	-0.803512000
1	3.432997000	-2.419762000	-0.275857000
6	-2.847055000	0.001599000	0.000816000
8	-3.309724000	-1.094275000	0.310635000
8	-3.296889000	1.104138000	-0.304747000
E = -643.553271945 N _{img} =0			

Im(NMe₂)₂-CO₂

At. No.	x	y	z
6	1.572030000	-0.002366000	0.000246000
7	0.785334000	-1.060297000	-0.054673000
7	0.787942000	1.057640000	0.055109000
6	-0.538719000	-0.683599000	-0.029995000
6	-0.536880000	0.684613000	0.028982000
1	1.193346000	-1.979664000	-0.103514000
1	1.199627000	1.975494000	0.103364000
7	-1.605405000	-1.558039000	-0.068340000
7	-1.600787000	1.562117000	0.069254000
6	-2.515837000	1.450921000	-1.048486000
1	-2.092324000	1.858088000	-1.971221000
1	-2.766137000	0.406789000	-1.211843000
1	-3.427559000	1.992458000	-0.812882000
6	-1.279025000	2.916437000	0.437410000
1	-0.706613000	2.927426000	1.361218000
1	-0.717100000	3.450017000	-0.338482000
1	-2.201470000	3.461415000	0.611942000
6	-2.512570000	-1.450521000	1.056211000
1	-2.083665000	-1.862702000	1.974220000
1	-2.760033000	-0.406697000	1.226015000
1	-3.426934000	-1.989246000	0.824334000
6	-1.289345000	-2.911190000	-0.445662000
1	-0.721027000	-2.918384000	-1.372017000
1	-0.725452000	-3.450885000	0.324594000

1	-2.214064000	-3.452711000	-0.619061000
6	3.093981000	-0.002341000	0.000095000
8	3.557986000	-1.139715000	-0.084994000
8	3.556764000	1.135580000	0.085128000
E = -682.418005023		N _{img} =0	

ImPh₂-CO₂

At. No.	x	y	z
6	-2.510798000	-0.000512000	0.000016000
7	-1.724354000	-1.058463000	0.014001000
7	-1.724761000	1.057738000	-0.013996000
6	-0.401261000	-0.683714000	0.015802000
6	-0.401515000	0.683500000	-0.015897000
1	-2.121413000	-1.982805000	0.069803000
1	-2.122200000	1.981917000	-0.069795000
6	0.686615000	-1.653934000	0.082420000
6	1.782926000	-1.417660000	0.905341000
6	0.628666000	-2.831575000	-0.655788000
6	2.808482000	-2.339842000	0.978821000
6	1.654630000	-3.755874000	-0.573451000
6	2.746996000	-3.510920000	0.240700000
1	1.822295000	-0.514738000	1.494774000
1	-0.210493000	-3.016450000	-1.310760000
1	3.652932000	-2.149451000	1.622587000
1	1.602020000	-4.664838000	-1.151992000
1	3.546860000	-4.232175000	0.302439000
6	0.685971000	1.654143000	-0.082443000
6	1.783013000	1.417804000	-0.904378000
6	0.626891000	2.832355000	0.654779000
6	2.808154000	2.340449000	-0.977817000
6	1.652439000	3.757114000	0.572467000
6	2.745537000	3.512080000	-0.240674000
1	1.823290000	0.514494000	-1.493144000
1	-0.212812000	3.017329000	1.309027000
1	3.653165000	2.149982000	-1.620825000
1	1.598924000	4.666509000	1.150248000
1	3.545074000	4.233698000	-0.302396000
6	-4.039973000	-0.000797000	0.000026000
8	-4.498615000	1.140028000	-0.022546000
8	-4.498194000	-1.141791000	0.022603000
E = -876.535224799		N _{img} =0	

ImF₂-CO₂

At. No.	x	y	z
6	-0.690959000	-0.000112000	0.000025000
7	0.090611000	1.065738000	-0.000091000

7	0.090756000	-1.065902000	0.000088000
6	1.396943000	0.673146000	-0.000126000
6	1.397046000	-0.673124000	-0.000020000
1	-0.306748000	1.994203000	-0.000149000
1	-0.306363000	-1.994454000	0.000201000
9	2.380723000	1.527255000	-0.000240000
9	2.380933000	-1.527090000	0.000000000
6	-2.227900000	-0.000041000	0.000095000
8	-2.672761000	-1.143338000	0.000538000
8	-2.672507000	1.143426000	-0.000253000
E = -613.014323242 N _{img} =0			

ImCl₂-CO₂

At. No.	x	y	z
6	-1.232052000	-0.000512000	0.000201000
7	-0.449427000	-1.063473000	0.000105000
7	-0.449902000	1.062729000	0.000219000
6	0.863566000	-0.677937000	-0.000001000
6	0.863274000	0.677865000	-0.000088000
1	-0.845723000	-1.991639000	0.000771000
1	-0.847123000	1.990546000	-0.000691000
17	2.149499000	1.760458000	0.000117000
17	2.150297000	-1.759927000	-0.000192000
6	-2.769809000	-0.000083000	0.000076000
8	-3.216577000	-1.142870000	0.000237000
8	-3.215705000	1.143028000	-0.000511000
E = -1333.89445259 N _{img} =0			

Im(CF₃)₂-CO₂

At. No.	x	y	z
6	1.847206000	-0.000443000	-0.000070000
7	1.061273000	-1.061024000	-0.013807000
7	1.061633000	1.060420000	0.013673000
6	-0.247895000	-0.677549000	-0.010164000
6	-0.247653000	0.677390000	0.009802000
1	1.452355000	-1.992464000	-0.039670000
1	1.453221000	1.991659000	0.039460000
6	-1.353864000	1.678732000	-0.003693000
9	-2.377958000	1.273770000	0.725111000
9	-0.902719000	2.826846000	0.492098000
9	-1.787166000	1.913463000	-1.233335000
6	-1.354460000	-1.678457000	0.003652000
9	-2.378936000	-1.272773000	-0.724171000
9	-0.904183000	-2.826562000	-0.492914000
9	-1.786908000	-1.913505000	1.233573000
6	3.389104000	-0.000278000	0.000005000

8	3.829760000	1.143337000	0.024510000
8	3.830277000	-1.143646000	-0.024423000
E = -1088.52068129		N _{img} =0	

Im(CN)₂-CO₂

At. No.	x	y	z
6	1.107423000	0.000084000	-0.000446000
7	0.325704000	-1.063200000	-0.000225000
7	0.325560000	1.063320000	-0.000302000
6	-0.987992000	-0.683436000	0.000013000
6	-0.988084000	0.683323000	-0.000032000
1	0.726232000	-1.991208000	0.000963000
1	0.725828000	1.991423000	-0.001016000
6	-2.072800000	-1.585536000	-0.000091000
7	-2.948296000	-2.331008000	-0.000179000
6	-2.072948000	1.585345000	0.000209000
7	-2.948188000	2.331119000	0.000476000
6	2.653654000	0.000053000	-0.000046000
8	3.089411000	1.144520000	-0.000232000
8	3.089209000	-1.144623000	0.000734000
E = -598.994722114		N _{img} =0	

Im(NO₂)₂-CO₂

At. No.	x	y	z
6	1.479986000	-0.000023000	0.000005000
7	0.693688000	1.063206000	-0.001695000
7	0.693664000	-1.063234000	0.001698000
6	-0.606726000	0.679799000	0.003053000
6	-0.606742000	-0.679796000	-0.003052000
1	1.059459000	2.007679000	-0.010110000
1	1.059391000	-2.007724000	0.010113000
7	-1.638994000	-1.676540000	-0.059889000
8	-1.271008000	-2.793250000	0.220200000
8	-2.733736000	-1.327120000	-0.398573000
7	-1.638964000	1.676556000	0.059881000
8	-1.270963000	2.793262000	-0.220205000
8	-2.733706000	1.327152000	0.398580000
6	3.031565000	-0.000010000	0.000002000
8	3.462619000	1.144869000	0.000719000
8	3.462656000	-1.144873000	-0.000723000
E = -823.411034669		N _{img} =0	

Im(CO₂Me)₂-CO₂

At. No.	x	y	z
6	-0.036353000	1.783640000	-0.000345000
7	1.038088000	1.018825000	0.001867000

7	-1.076813000	0.973339000	-0.002654000
6	0.692365000	-0.303853000	0.000490000
6	-0.675230000	-0.332878000	-0.001646000
1	1.968360000	1.409167000	0.000626000
1	-2.022915000	1.324160000	-0.001045000
6	-1.669388000	-1.422904000	-0.003057000
8	-1.428446000	-2.590827000	-0.001597000
8	-2.889192000	-0.895387000	-0.003558000
6	-3.957832000	-1.835230000	-0.003293000
1	-3.902095000	-2.460028000	-0.888145000
1	-3.902287000	-2.459322000	0.882070000
1	-4.864609000	-1.246439000	-0.003619000
6	1.729788000	-1.352297000	0.001800000
8	1.535062000	-2.528907000	0.000880000
8	2.927308000	-0.775895000	0.004038000
6	4.034028000	-1.670378000	0.005243000
1	4.003265000	-2.296991000	0.890028000
1	4.005964000	-2.295968000	-0.880358000
1	4.915387000	-1.044093000	0.006950000
6	-0.073236000	3.321512000	0.000096000
8	1.056792000	3.799016000	-0.033470000
8	-1.225881000	3.741836000	0.034115000
E = -870.184109986 N _{img} =0			

ImNMe₂-CO₂

At. No.	x	y	z
6	-0.000007000	0.088138000	-0.000443000
7	1.073805000	-0.703580000	-0.000245000
6	-0.674701000	-2.008550000	0.000582000
7	-1.073659000	-0.703796000	-0.000249000
6	0.675109000	-2.008414000	0.000624000
6	-2.463435000	-0.277405000	-0.000555000
6	2.463498000	-0.276915000	-0.000566000
1	2.665959000	0.320265000	0.878225000
1	3.073930000	-1.172679000	-0.009084000
1	-2.666094000	0.319463000	0.878404000
1	-3.073692000	-1.173285000	-0.009400000
1	-1.375638000	-2.819438000	0.000885000
1	1.376209000	-2.819160000	0.000964000
6	-0.000168000	1.628293000	0.000082000
8	-1.133794000	2.103452000	0.000394000
8	1.133356000	2.103694000	0.000392000
1	2.660848000	0.334334000	-0.870679000
1	-2.660820000	0.334079000	-0.870494000
E = -493.190796435 N _{img} =0			

ImNEt₂-CO₂

At. No.	x	y	z
6	0.000012000	0.105277000	-0.000037000
7	1.031329000	-0.687012000	-0.300621000
6	-0.647451000	-1.992269000	0.189168000
7	-1.031266000	-0.687055000	0.300557000
6	0.647517000	-1.992244000	-0.189416000
6	-2.385592000	-0.274807000	0.664481000
6	-3.258766000	-0.095601000	-0.552993000
6	2.385705000	-0.274727000	-0.664325000
6	3.258713000	-0.095558000	0.553269000
1	3.310671000	-1.006410000	1.145882000
1	2.867953000	0.716642000	1.157107000
1	4.266322000	0.164582000	0.240173000
1	-4.266299000	0.164652000	-0.239752000
1	-3.310904000	-1.006469000	-1.145563000
1	-2.868044000	0.716542000	-1.156925000
1	2.764955000	-1.052028000	-1.322645000
1	2.305811000	0.655288000	-1.211043000
1	-2.305652000	0.655187000	1.211232000
1	-2.764724000	-1.052148000	1.322822000
1	-1.320953000	-2.802088000	0.389213000
1	1.321027000	-2.802031000	-0.389564000
6	-0.000047000	1.648956000	-0.000043000
8	-1.130362000	2.130726000	-0.047356000
8	1.130218000	2.130848000	0.047218000
E =	-571.784850045	N _{img} =0	

ImNⁱPr₂-CO₂

At. No.	x	y	z
6	-0.000005000	0.298362000	-0.000220000
7	-1.072051000	-0.490564000	0.092742000
7	1.072165000	-0.490446000	-0.092983000
6	-0.671392000	-1.797140000	0.057630000
6	0.671559000	-1.797059000	-0.058725000
6	-2.471237000	-0.041584000	0.175038000
6	2.471385000	-0.041387000	-0.174630000
6	-3.243595000	-0.913388000	1.140150000
6	-3.071077000	-0.011115000	-1.212802000
6	3.244208000	-0.913114000	-1.139440000
6	3.070672000	-0.010985000	1.213449000
1	-1.360755000	-2.614148000	0.122339000
1	1.360970000	-2.613996000	-0.123830000
1	-2.419206000	0.973602000	0.548320000
1	-2.510838000	0.679085000	-1.835242000
1	-4.099914000	0.334948000	-1.157963000

1	-3.068973000	-1.002802000	-1.663252000
1	-2.744316000	-0.984262000	2.103048000
1	-4.223046000	-0.472146000	1.299987000
1	-3.404391000	-1.917676000	0.752268000
1	2.419534000	0.973803000	-0.547919000
1	3.068438000	-1.002712000	1.663795000
1	2.510126000	0.679155000	1.835665000
1	4.099517000	0.335140000	1.159031000
1	3.405177000	-1.917310000	-0.751391000
1	4.223599000	-0.471653000	-1.299065000
1	2.745228000	-0.984227000	-2.102474000
6	-0.000164000	1.841464000	-0.000223000
8	-1.002782000	2.324084000	-0.524731000
8	1.002274000	2.324408000	0.524357000
E = -650.374723194 N _{img} =0			

ImNcy₂-CO₂

At. No.	x	y	z
6	-0.004173000	0.312897000	-0.175704000
7	1.081250000	-0.446777000	-0.021322000
7	-1.068844000	-0.487956000	-0.092075000
6	0.697618000	-1.745271000	0.172340000
6	-0.648898000	-1.771461000	0.124455000
6	2.469981000	0.018901000	0.000030000
6	3.103890000	-0.276430000	1.346064000
6	4.534182000	0.232777000	1.366458000
6	5.343237000	-0.371188000	0.232972000
6	4.691131000	-0.094292000	-1.109407000
6	3.257594000	-0.595877000	-1.140901000
6	-2.470416000	-0.063496000	-0.167994000
6	-3.034912000	0.131286000	1.225863000
6	-4.467551000	0.624844000	1.136515000
6	-5.326481000	-0.312920000	0.307425000
6	-4.728831000	-0.524980000	-1.072616000
6	-3.301307000	-1.038157000	-0.978091000
1	1.403923000	-2.536121000	0.326776000
1	-1.329615000	-2.592471000	0.220701000
1	2.406843000	1.090671000	-0.160693000
1	2.515969000	0.184003000	2.138283000
1	3.104740000	-1.354304000	1.527701000
1	4.527660000	1.319657000	1.268375000
1	4.992261000	0.007972000	2.327781000
1	6.359495000	0.018767000	0.245585000
1	5.420450000	-1.451037000	0.381507000
1	4.694298000	0.979909000	-1.300517000
1	5.259674000	-0.556280000	-1.914306000

1	2.778294000	-0.342100000	-2.083966000
1	3.251642000	-1.685562000	-1.049010000
1	-2.451662000	0.903503000	-0.660340000
1	-2.411123000	0.848980000	1.752172000
1	-2.999475000	-0.819720000	1.764474000
1	-4.466587000	1.617420000	0.683482000
1	-4.881189000	0.739549000	2.136608000
1	-5.405184000	-1.276954000	0.815955000
1	-6.339168000	0.077272000	0.221332000
1	-4.734481000	0.419443000	-1.619435000
1	-5.332400000	-1.223990000	-1.648643000
1	-3.317240000	-2.017313000	-0.494151000
1	-2.867838000	-1.170201000	-1.968482000
6	-0.034859000	1.841497000	-0.393846000
8	0.912875000	2.263298000	-1.054987000
8	-1.006293000	2.380858000	0.135137000
E = -883.749706682 N _{img} =0			

ImN(OMe)₂-CO₂

At. No.	x	y	z
6	0.000063000	0.114215000	-0.000088000
7	-1.010516000	-0.705129000	-0.279534000
7	1.010647000	-0.705199000	0.279184000
6	-0.648097000	-2.019390000	-0.187615000
6	0.648144000	-2.019406000	0.187529000
1	1.335175000	-2.811764000	0.405550000
1	-1.335161000	-2.811706000	-0.405664000
8	2.214567000	-0.310409000	0.727491000
6	3.113069000	-0.033008000	-0.352749000
1	3.277056000	-0.935118000	-0.937821000
1	2.715213000	0.780157000	-0.948307000
1	4.030705000	0.265044000	0.138009000
8	-2.214613000	-0.310456000	-0.727419000
6	-3.112832000	-0.033159000	0.353103000
1	-3.275365000	-0.934923000	0.939071000
1	-2.715535000	0.780954000	0.947657000
1	-4.031154000	0.263248000	-0.137369000
6	-0.000117000	1.672817000	-0.000054000
8	0.982422000	2.134617000	-0.566072000
8	-0.982781000	2.134246000	0.566072000
E = -643.427634930 N _{img} =0			

ImN(NMe₂)₂-CO₂

At. No.	x	y	z
6	0.000002000	0.003851000	0.000020000
7	1.063762000	0.810491000	-0.075603000

7	-1.063764000	0.810486000	0.075581000
6	0.670359000	2.121874000	-0.057858000
6	-0.670375000	2.121871000	0.057756000
1	-1.391605000	2.910251000	0.130979000
1	1.391584000	2.910257000	-0.131101000
7	-2.411361000	0.488782000	0.187755000
7	2.411357000	0.488783000	-0.187752000
6	-2.680540000	-0.437271000	1.271821000
1	-3.751160000	-0.414892000	1.451907000
1	-2.378097000	-1.459103000	1.047885000
1	-2.178638000	-0.088848000	2.169106000
6	-2.986808000	0.096647000	-1.090491000
1	-4.061543000	0.034314000	-0.947907000
1	-2.788732000	0.877584000	-1.818943000
1	-2.593910000	-0.855927000	-1.442719000
6	2.986779000	0.096751000	1.090532000
1	4.061459000	0.033791000	0.947803000
1	2.789244000	0.878021000	1.818775000
1	2.593479000	-0.855542000	1.443073000
6	2.680554000	-0.437341000	-1.271761000
1	2.178388000	-0.089139000	-2.168984000
1	3.751131000	-0.414732000	-1.452069000
1	2.378362000	-1.459209000	-1.047653000
6	0.000013000	-1.540973000	0.000003000
8	-0.852270000	-2.021798000	-0.741775000
8	0.852293000	-2.021837000	0.741755000
E = -682.343176223 N _{img} =0			

ImNPh₂-CO₂

At. No.	x	y	z
6	0.000030000	0.001879000	-0.046110000
7	-1.072437000	0.758852000	-0.281161000
7	1.072598000	0.758686000	-0.281258000
6	-0.670964000	2.019741000	-0.663980000
6	0.671258000	2.019646000	-0.664020000
1	1.377486000	2.778596000	-0.934018000
1	-1.377105000	2.778770000	-0.933985000
6	-2.429214000	0.359736000	-0.125980000
6	-2.850079000	-0.864990000	-0.610763000
6	-3.303273000	1.228973000	0.503018000
6	-4.179002000	-1.217169000	-0.453872000
6	-4.630675000	0.868763000	0.638769000
6	-5.069679000	-0.354839000	0.161621000
1	-2.143513000	-1.532303000	-1.080378000
1	-2.943506000	2.163763000	0.904880000
1	-4.515599000	-2.174053000	-0.820078000

1	-5.316794000	1.538191000	1.133138000
1	-6.104043000	-0.638467000	0.276528000
6	2.429368000	0.359571000	-0.125920000
6	3.303357000	1.228927000	0.503028000
6	2.850300000	-0.865212000	-0.610501000
6	4.630764000	0.868790000	0.638918000
6	4.179239000	-1.217297000	-0.453480000
6	5.069849000	-0.354854000	0.161948000
1	2.943536000	2.163762000	0.904738000
1	2.143732000	-1.532621000	-1.079977000
1	5.316823000	1.538313000	1.133243000
1	4.515900000	-2.174213000	-0.819547000
1	6.104219000	-0.638421000	0.276947000
6	-0.000307000	-1.464660000	0.438708000
8	-0.002010000	-1.562695000	1.655820000
8	0.001000000	-2.261819000	-0.502429000
E = -876.497376921 N _{img} =0			

ImNMes₂-CO₂

At. No.	x	y	z
6	0.001281000	0.066014000	0.106195000
7	1.070741000	0.107210000	0.893249000
7	-1.072470000	0.089856000	0.888329000
6	0.669033000	0.157377000	2.209128000
6	-0.676428000	0.149567000	2.206145000
1	-1.389107000	0.179597000	3.006118000
1	1.377741000	0.189505000	3.012522000
6	2.420844000	0.035482000	0.429497000
6	2.974802000	-1.220550000	0.229003000
6	3.097643000	1.219172000	0.166268000
6	4.289220000	-1.271198000	-0.209149000
6	4.407877000	1.114266000	-0.269146000
6	5.020018000	-0.118463000	-0.453477000
1	4.745190000	-2.236022000	-0.378599000
1	4.957967000	2.018254000	-0.488756000
6	-2.422717000	0.033694000	0.422950000
6	-3.081087000	1.225810000	0.155091000
6	-3.004039000	-1.214501000	0.246583000
6	-4.396015000	1.141311000	-0.273804000
6	-4.319969000	-1.244801000	-0.185066000
6	-5.028825000	-0.081093000	-0.447585000
1	-4.933744000	2.053516000	-0.489697000
1	-4.798236000	-2.202668000	-0.331844000
6	-2.374983000	2.535915000	0.286127000
1	-1.541233000	2.583888000	-0.413555000
1	-3.049875000	3.358062000	0.071544000

1	-1.974819000	2.679622000	1.288361000
6	-2.215104000	-2.462810000	0.467606000
1	-2.845590000	-3.339923000	0.364018000
1	-1.414169000	-2.519407000	-0.269281000
1	-1.761960000	-2.485006000	1.457462000
6	-6.436086000	-0.144817000	-0.950084000
1	-7.003629000	0.732017000	-0.651115000
1	-6.451131000	-0.190568000	-2.037939000
1	-6.949725000	-1.026830000	-0.578011000
6	2.404505000	2.536111000	0.290215000
1	3.089829000	3.351655000	0.083128000
1	1.581168000	2.581459000	-0.423421000
1	1.993533000	2.683939000	1.287500000
6	2.159354000	-2.457840000	0.421722000
1	1.361820000	-2.494657000	-0.320908000
1	2.774839000	-3.344505000	0.309668000
1	1.696805000	-2.488684000	1.406967000
6	6.443493000	-0.195365000	-0.906242000
1	6.680708000	-1.179266000	-1.299831000
1	6.649189000	0.538130000	-1.681475000
1	7.123712000	0.003841000	-0.079558000
6	0.017077000	0.022795000	-1.428802000
8	0.186246000	1.137180000	-1.919471000
8	-0.137065000	-1.109914000	-1.879704000
E = -1112.28268468 N _{img} =0			

ImN(CO₂Me)₂-CO₂

At. No.	x	y	z
6	-0.000064000	0.082936000	-0.000032000
7	1.063384000	0.898246000	-0.000031000
7	-1.063525000	0.898217000	-0.000008000
6	0.666596000	2.228714000	0.000031000
6	-0.666781000	2.228695000	0.000045000
1	-1.392027000	3.016805000	0.000084000
1	1.391856000	3.016814000	0.000045000
6	-2.438285000	0.543301000	-0.000022000
8	-3.281131000	1.389373000	0.001128000
8	-2.582665000	-0.741597000	-0.001471000
6	-3.919035000	-1.233010000	-0.001044000
1	-4.435808000	-0.889116000	0.887905000
1	-4.436810000	-0.887919000	-0.888949000
1	-3.820633000	-2.308934000	-0.001809000
6	2.438134000	0.543364000	-0.000178000
8	3.280950000	1.389478000	-0.001008000
8	2.582616000	-0.741531000	0.000794000
6	3.919084000	-1.232735000	0.000359000

1	4.436219000	-0.887590000	-0.887890000
1	4.436333000	-0.888683000	0.888973000
1	3.820856000	-2.308672000	-0.000268000
6	0.000115000	-1.485267000	0.000415000
8	-0.001796000	-1.928303000	1.137471000
8	0.002327000	-1.929161000	-1.136321000
E = -870.159353840		N _{img} =0	

Im(NO₂)₂NMe₂-CO₂

At. No.	x	y	z
6	1.349745000	-0.000012000	-0.000092000
7	0.565470000	1.082566000	-0.047148000
7	0.565441000	-1.082576000	0.046937000
6	-0.730329000	0.674770000	-0.033147000
6	-0.730349000	-0.674740000	0.032963000
7	-1.845046000	-1.570645000	0.137387000
8	-1.719876000	-2.644460000	-0.398658000
8	-2.794897000	-1.171717000	0.756915000
7	-1.845025000	1.570692000	-0.137344000
8	-1.719658000	2.644579000	0.398504000
8	-2.795097000	1.171694000	-0.756498000
6	1.032836000	-2.464704000	0.165682000
1	0.771154000	-3.000263000	-0.736693000
1	2.106601000	-2.426183000	0.275901000
1	0.551943000	-2.923206000	1.021384000
6	1.032962000	2.464665000	-0.165942000
1	0.771518000	3.000197000	0.736524000
1	2.106688000	2.426077000	-0.276438000
1	0.551867000	2.923261000	-1.021475000
6	2.918896000	-0.000035000	0.000108000
8	3.377924000	0.969746000	0.587812000
8	3.378077000	-0.969818000	-0.587507000
E = -901.985012089		N _{img} =0	

Im(CF₃)₂NMe₂-CO₂

At. No.	x	y	z
7	-0.867853000	-1.073985000	0.049797000
7	-0.867902000	1.073914000	-0.050067000
6	-1.653399000	-0.000064000	-0.000137000
6	-1.342156000	-2.450679000	0.170983000
6	0.442322000	-0.677905000	0.019574000
6	0.442272000	0.677899000	-0.019817000
6	-1.342280000	2.450592000	-0.171016000
1	-2.335538000	-2.423714000	0.591576000
1	-2.335486000	2.423691000	-0.592023000
1	-1.392807000	-2.905799000	-0.809857000

1	-0.658881000	-2.994797000	0.809944000
1	-1.393339000	2.905419000	0.809936000
1	-0.658884000	2.994958000	-0.809632000
6	1.538562000	1.694428000	0.001365000
6	1.538682000	-1.694357000	-0.001382000
9	2.677074000	1.195704000	0.436208000
9	1.741036000	2.212781000	-1.207026000
9	1.206318000	2.696938000	0.811038000
9	2.677101000	-1.195716000	-0.436555000
9	1.741325000	-2.212234000	1.207178000
9	1.206432000	-2.697215000	-0.810640000
6	-3.210215000	-0.000060000	0.000064000
8	-3.674947000	1.013838000	0.508687000
8	-3.675188000	-1.013927000	-0.508400000
E = -1167.09123965 N _{img} =0			

ImNMe₂N(Me)₂-CO₂

At. No.	x	y	z
7	-0.751360000	1.097641000	-0.082719000
7	-0.609076000	-1.042621000	-0.004692000
6	-1.467622000	-0.028348000	-0.025630000
6	-1.272284000	2.448814000	-0.157803000
6	0.592599000	0.794196000	-0.085622000
6	0.691475000	-0.561326000	-0.035507000
6	-0.955036000	-2.450369000	0.004856000
1	-2.190177000	2.426370000	-0.728607000
1	-0.944488000	-2.839638000	-1.009160000
1	-1.486605000	2.823408000	0.839063000
1	-0.508825000	3.059323000	-0.625714000
1	-0.225049000	-2.981290000	0.603860000
1	-1.947595000	-2.542636000	0.426816000
6	2.098652000	-2.205216000	-1.124332000
1	1.600264000	-3.177145000	-1.054550000
1	1.780438000	-1.720130000	-2.042258000
1	3.170003000	-2.387084000	-1.191291000
6	1.782327000	2.501927000	1.076829000
1	2.361727000	1.903734000	1.787411000
1	2.330846000	3.416110000	0.865492000
1	0.840386000	2.773755000	1.543397000
7	1.541793000	1.794448000	-0.162936000
7	1.832815000	-1.340161000	-0.001113000
6	2.754371000	1.468763000	-0.876911000
1	3.271964000	2.395158000	-1.113960000
1	3.425590000	0.823809000	-0.306038000
1	2.505323000	0.968234000	-1.807390000
6	2.253509000	-1.861556000	1.277133000

1	1.746080000	-2.790659000	1.557276000
1	3.322629000	-2.064846000	1.246078000
1	2.068774000	-1.124217000	2.051591000
6	-3.013475000	-0.122957000	0.009380000
8	-3.570876000	0.823167000	-0.542364000
8	-3.430072000	-1.127039000	0.585344000
E = -760.987786346		N _{img} =0	

ImCl₂NMe₂-CO₂

At. No.	x	y	z
7	0.302905000	1.076891000	-0.021662000
7	0.302926000	-1.076870000	0.021703000
6	1.093689000	0.000015000	0.000010000
6	0.717983000	2.469251000	-0.081325000
6	-1.004869000	0.674362000	-0.017525000
6	-1.004856000	-0.674378000	0.017505000
6	0.718064000	-2.469205000	0.081449000
1	1.793496000	2.488507000	0.034296000
1	1.793573000	-2.488416000	-0.034217000
1	0.410120000	2.890549000	-1.032375000
1	0.242840000	3.008744000	0.730185000
1	0.410266000	-2.890456000	1.032541000
1	0.242915000	-3.008772000	-0.730007000
17	-2.302711000	-1.746145000	0.059657000
17	-2.302747000	1.746101000	-0.059688000
6	2.654748000	0.000007000	-0.000018000
8	3.131859000	-1.023804000	-0.477896000
8	3.131917000	1.023819000	0.477801000
E = -1412.47082545		N _{img} =0	

Im(CN)₂NMe₂-CO₂

At. No.	x	y	z
7	0.182022000	1.076752000	0.023670000
7	0.181864000	-1.076500000	-0.023762000
6	0.971000000	0.000015000	0.000161000
6	0.606996000	2.469559000	0.089873000
6	-1.125839000	0.680581000	0.020324000
6	-1.125951000	-0.680165000	-0.020076000
6	0.605936000	-2.469599000	-0.089766000
1	1.653610000	2.498611000	-0.184540000
1	1.653920000	-2.498686000	0.179280000
1	0.008372000	3.044064000	-0.607244000
1	0.456543000	2.838350000	1.098791000
1	0.010744000	-3.042287000	0.611831000
1	0.449397000	-2.840232000	-1.097070000
6	-2.209391000	-1.582742000	-0.055896000

6	-2.209480000	1.582933000	0.056257000
7	-3.082056000	-2.331733000	-0.085188000
7	-3.082169000	2.331927000	0.084700000
6	2.538249000	-0.000294000	-0.000160000
8	3.003678000	-0.993213000	0.543653000
8	3.003904000	0.992628000	-0.543813000
E = -677.574744181		N _{img} =0	

Im(CO₂Me)₂NMe₂-CO₂

At. No.	x	y	z
8	-2.525920000	0.953284000	-0.706501000
8	-1.344402000	2.639075000	0.154820000
8	-1.323291000	-2.725323000	-0.865742000
8	-2.282553000	-1.511153000	0.744900000
7	1.003985000	1.017171000	-0.026110000
7	1.069378000	-1.137140000	-0.030063000
6	1.821816000	-0.034247000	0.013441000
6	1.443990000	2.405606000	-0.061509000
6	-0.294139000	0.575131000	-0.091843000
6	-1.506078000	1.392131000	-0.252216000
6	-2.486725000	3.475456000	0.014681000
6	1.563683000	-2.506475000	0.036949000
6	-0.245746000	-0.781730000	-0.077086000
6	-1.337919000	-1.779542000	-0.128301000
6	-3.426274000	-2.353509000	0.682983000
1	-4.088062000	-2.003202000	1.462857000
1	-2.176090000	4.453018000	0.357214000
1	-3.896983000	-2.261409000	-0.290111000
1	-3.141134000	-3.386383000	0.852167000
1	-2.799783000	3.509838000	-1.023324000
1	-3.301284000	3.096160000	0.622231000
1	1.029197000	2.884215000	-0.940279000
1	2.524046000	2.403110000	-0.074351000
1	1.093535000	2.911554000	0.828470000
1	1.094892000	-3.079850000	-0.751553000
1	1.309183000	-2.928729000	1.003665000
1	2.635763000	-2.465684000	-0.101422000
6	3.374741000	0.012121000	0.113097000
8	3.774771000	0.941413000	0.807620000
8	3.921281000	-0.887609000	-0.516788000
E = -948.752623091		N _{img} =0	

ImF₂NMe₂-CO₂

At. No.	x	y	z
7	0.166380000	1.076421000	0.022391000
7	0.166378000	-1.076399000	-0.022263000

6	-0.628887000	0.000013000	0.000100000
6	-0.213580000	2.481415000	0.085031000
6	1.465468000	0.669655000	0.016815000
6	1.465454000	-0.669642000	-0.016853000
6	-0.213538000	-2.481405000	-0.084866000
1	-1.284008000	2.527522000	-0.064843000
1	-1.284452000	-2.527223000	0.061657000
1	0.067668000	2.880422000	1.053501000
1	0.311132000	3.015188000	-0.698867000
1	0.070929000	-2.881252000	-1.052051000
1	0.308442000	-3.014611000	0.701246000
9	2.446398000	-1.531794000	-0.046492000
9	2.446452000	1.531762000	0.046427000
6	-2.188959000	-0.000002000	-0.000068000
8	-2.666933000	-1.078238000	0.335947000
8	-2.666870000	1.078224000	-0.336186000
E = -691.591657034 N _{img} =0			

ImMe₂NMe₂-CO₂

At. No.	x	y	z
7	0.121641000	-1.069468000	-0.029951000
7	0.121668000	1.069524000	0.029796000
6	-0.674237000	0.000036000	-0.000090000
6	-0.296230000	-2.455216000	-0.105922000
6	1.440414000	-0.676448000	-0.023761000
6	1.440427000	0.676473000	0.023582000
6	-0.296153000	2.455309000	0.105087000
1	-1.369882000	-2.484636000	0.027326000
1	-1.370027000	2.484569000	-0.026392000
1	-0.009843000	-2.867278000	-1.069162000
1	0.189984000	-3.015034000	0.686535000
1	-0.008038000	2.868406000	1.067346000
1	0.188478000	3.014350000	-0.688908000
6	2.553216000	1.648873000	0.066967000
1	2.503655000	2.272612000	0.957294000
1	3.503780000	1.127216000	0.078877000
1	2.543982000	2.307310000	-0.799481000
6	2.553138000	-1.648956000	-0.066461000
1	2.546681000	-2.303733000	0.802817000
1	2.500801000	-2.276423000	-0.953970000
1	3.503640000	-1.127324000	-0.083612000
6	-2.224299000	-0.000010000	0.000182000
8	-2.712933000	1.024459000	-0.472565000
8	-2.712570000	-1.024558000	0.473179000
E = -571.790749876 N _{img} =0			

ImMe₂N(OMe)₂-CO₂

At. No.	x	y	z
6	0.000013000	-0.609223000	0.000107000
7	-1.020816000	0.210963000	0.223028000
7	1.020774000	0.211019000	-0.223013000
6	-0.659896000	1.537533000	0.154744000
6	0.659764000	1.537547000	-0.154908000
8	2.240945000	-0.183088000	-0.629260000
6	3.099723000	-0.456924000	0.481193000
1	3.238249000	0.443687000	1.075787000
1	2.683041000	-1.270661000	1.062007000
1	4.037735000	-0.750651000	0.027253000
8	-2.240909000	-0.183310000	0.629376000
6	-3.099871000	-0.457134000	-0.480937000
1	-3.238714000	0.443492000	-1.075431000
1	-2.683149000	-1.270700000	-1.061956000
1	-4.037750000	-0.751118000	-0.026890000
6	0.000118000	-2.163844000	-0.000067000
8	0.949540000	-2.630010000	0.619216000
8	-0.949282000	-2.629935000	-0.619444000
6	-1.628468000	2.621690000	0.414862000
1	-2.108857000	2.481180000	1.379428000
1	-1.122126000	3.580395000	0.417061000
1	-2.407842000	2.651044000	-0.343228000
6	1.628393000	2.621660000	-0.414954000
1	2.108862000	2.481065000	-1.379465000
1	1.122121000	3.580397000	-0.417219000
1	2.407716000	2.650910000	0.343202000
E = -722.031326781 N _{img} =0			

ImMe₂N(NMe₂)₂-CO₂

At. No.	x	y	z
6	0.000017000	-0.435564000	-0.000011000
7	-1.062060000	0.369592000	0.060267000
7	1.062042000	0.369655000	-0.060276000
6	-0.674338000	1.694752000	0.048201000
6	0.674248000	1.694793000	-0.048213000
7	2.405016000	0.036696000	-0.163900000
7	-2.405026000	0.036585000	0.163895000
6	2.680818000	-0.895250000	-1.240392000
1	3.751866000	-0.871003000	-1.419841000
1	2.381510000	-1.916873000	-1.011110000
1	2.177806000	-0.556393000	-2.140839000
6	2.973482000	-0.345255000	1.119217000
1	4.049039000	-0.416358000	0.985128000
1	2.775190000	0.442466000	1.841257000

1	2.571420000	-1.291455000	1.479126000
6	-2.973487000	-0.345413000	-1.119209000
1	-4.049043000	-0.416530000	-0.985116000
1	-2.775211000	0.442290000	-1.841272000
1	-2.571415000	-1.291619000	-1.479089000
6	-2.680835000	-0.895306000	1.240437000
1	-2.177861000	-0.556377000	2.140879000
1	-3.751888000	-0.871072000	1.419851000
1	-2.381500000	-1.916937000	1.011232000
6	0.000088000	-1.977108000	-0.000005000
8	0.833584000	-2.461718000	0.762252000
8	-0.833361000	-2.461824000	-0.762246000
6	1.659735000	2.791111000	-0.135481000
1	2.324464000	2.799705000	0.724936000
1	2.278999000	2.681172000	-1.021179000
1	1.147681000	3.746226000	-0.182234000
6	-1.659891000	2.791013000	0.135450000
1	-2.324634000	2.799535000	-0.724958000
1	-2.279134000	2.681067000	1.021161000
1	-1.147895000	3.746161000	0.182160000
E = -760.945515825 N _{img} =0			

ImEt₂N(OMe)₂-CO₂

At. No.	x	y	z
6	0.185152000	0.954119000	-0.001164000
7	-0.997088000	0.346815000	-0.026800000
7	1.055042000	-0.050756000	0.023089000
6	-0.888575000	-1.026070000	-0.026023000
6	0.442153000	-1.283393000	0.022700000
8	2.386957000	0.090965000	0.155664000
6	3.024758000	0.274518000	-1.112770000
1	2.840159000	-0.588667000	-1.749069000
1	2.671539000	1.196083000	-1.560551000
1	4.078544000	0.341980000	-0.872925000
8	-2.177954000	0.978133000	-0.163041000
6	-2.712814000	1.369172000	1.105088000
1	-2.889482000	0.490563000	1.722003000
1	-2.035215000	2.069502000	1.577522000
1	-3.652459000	1.848853000	0.861470000
6	0.480903000	2.480312000	0.002994000
8	1.371730000	2.786423000	-0.781330000
8	-0.230890000	3.093308000	0.790202000
6	1.211194000	-2.545708000	0.135109000
1	0.556643000	-3.365355000	-0.150776000
1	2.025137000	-2.534868000	-0.587886000
6	1.769369000	-2.772525000	1.532505000

1	0.968945000	-2.832682000	2.265263000
1	2.430857000	-1.959492000	1.816796000
1	2.334013000	-3.700265000	1.569371000
6	-2.072047000	-1.912628000	-0.131523000
1	-1.767602000	-2.915084000	0.159030000
1	-2.821519000	-1.597287000	0.592312000
6	-2.679912000	-1.925570000	-1.526420000
1	-1.961963000	-2.283811000	-2.259506000
1	-2.994692000	-0.927686000	-1.817298000
1	-3.548404000	-2.578201000	-1.554714000
E = -800.616606750 N _{img} =0			

ImEt₂N(NMe₂)₂-CO₂

At. No.	x	y	z
6	0.000228000	-0.783441000	-0.000135000
7	-1.060733000	0.020703000	-0.075402000
7	1.060875000	0.021142000	0.075225000
6	-0.675083000	1.347515000	-0.039641000
6	0.674675000	1.347778000	0.039928000
7	2.402044000	-0.316654000	0.177764000
7	-2.401753000	-0.317590000	-0.178163000
6	2.831355000	-1.283084000	-0.813458000
1	3.917538000	-1.268137000	-0.827257000
1	2.493094000	-2.296136000	-0.601368000
1	2.473485000	-0.972616000	-1.790571000
6	2.775929000	-0.645562000	1.542608000
1	3.859159000	-0.720416000	1.571890000
1	2.475475000	0.169438000	2.196081000
1	2.324660000	-1.576488000	1.877522000
6	-2.775337000	-0.646815000	-1.542922000
1	-3.858514000	-0.722491000	-1.572305000
1	-2.475470000	0.168331000	-2.196490000
1	-2.323523000	-1.577479000	-1.877870000
6	-2.831100000	-1.283571000	0.813460000
1	-2.473836000	-0.972279000	1.790530000
1	-3.917295000	-1.269127000	0.826724000
1	-2.492384000	-2.296650000	0.602224000
6	0.000558000	-2.325959000	0.000097000
8	0.657739000	-2.809124000	0.919844000
8	-0.656470000	-2.809865000	-0.919299000
6	1.663432000	2.451825000	0.052718000
1	1.143735000	3.368579000	0.321478000
1	2.395947000	2.262681000	0.834918000
6	2.376225000	2.619734000	-1.280307000
1	1.669256000	2.844836000	-2.074961000
1	2.907748000	1.708650000	-1.540215000

1	3.098514000	3.430431000	-1.228490000
6	-1.664222000	2.451203000	-0.052399000
1	-1.144722000	3.368304000	-0.320387000
1	-2.396116000	2.262339000	-0.835266000
6	-2.378029000	2.618341000	1.280146000
1	-1.671746000	2.843451000	2.075408000
1	-2.909351000	1.706964000	1.539443000
1	-3.100628000	3.428739000	1.228072000
E = -839.530503665		N _{img} =0	

ImPh₂N(OMe)₂-CO₂

At. No.	x	y	z
6	-2.133349000	-0.037800000	0.005730000
7	-1.344278000	1.028012000	-0.070292000
7	-1.293356000	-1.059983000	0.109020000
6	-0.007114000	0.696046000	-0.027326000
6	0.025052000	-0.662704000	0.088772000
8	-1.689639000	-2.330340000	0.297601000
6	-1.825246000	-3.024241000	-0.945978000
1	-2.574841000	-2.526561000	-1.549353000
1	-0.858310000	-3.083300000	-1.440266000
1	-2.161136000	-4.013725000	-0.662702000
8	-1.795036000	2.283883000	-0.233133000
6	-2.121666000	2.886177000	1.025918000
1	-2.925748000	2.322179000	1.489950000
1	-1.229688000	2.942092000	1.645733000
1	-2.455616000	3.882049000	0.763094000
6	1.149549000	-1.595700000	0.094856000
6	2.182770000	-1.406393000	-0.818319000
6	1.208165000	-2.663924000	0.983937000
6	3.261310000	-2.268743000	-0.838776000
6	2.289693000	-3.526600000	0.955802000
6	3.316561000	-3.331939000	0.047563000
1	2.134623000	-0.580854000	-1.512134000
1	0.408324000	-2.815604000	1.691037000
1	4.055719000	-2.114876000	-1.552255000
1	2.329565000	-4.352087000	1.649305000
1	4.156939000	-4.008365000	0.029561000
6	1.079775000	1.670868000	-0.056332000
6	2.155794000	1.501850000	0.810492000
6	1.076815000	2.744604000	-0.941640000
6	3.217219000	2.384931000	0.785400000
6	2.140450000	3.629318000	-0.957082000
6	3.212036000	3.451478000	-0.098563000
1	2.156862000	0.673473000	1.502428000
1	0.246719000	2.880680000	-1.615879000

1	4.046535000	2.243743000	1.460723000
1	2.132200000	4.457444000	-1.648562000
1	4.039820000	4.143227000	-0.117623000
6	-3.687124000	-0.086806000	-0.056083000
8	-4.086281000	-0.932881000	-0.847203000
8	-4.214376000	0.730807000	0.688438000
E = -1105.34559526		N _{img} =0	

ImPh₂N(NMe₂)₂-CO₂

At. No.	x	y	z
6	1.889881000	-0.000026000	0.000442000
7	1.092288000	1.067082000	-0.020020000
7	1.092323000	-1.066776000	0.021833000
6	-0.235615000	0.679407000	-0.016158000
6	-0.235502000	-0.679399000	0.018351000
7	1.457632000	-2.403922000	0.008653000
7	1.457174000	2.404203000	-0.005757000
6	2.449051000	-2.739341000	1.011427000
1	2.439921000	-3.820123000	1.122037000
1	3.456017000	-2.418017000	0.748747000
1	2.160727000	-2.297250000	1.960623000
6	1.767471000	-2.867390000	-1.333328000
1	1.894163000	-3.944506000	-1.277830000
1	0.917695000	-2.663172000	-1.978853000
1	2.669352000	-2.401023000	-1.728245000
6	1.769579000	2.866294000	1.335832000
1	1.893801000	3.943897000	1.282365000
1	0.922174000	2.659008000	1.983581000
1	2.673475000	2.401438000	1.728185000
6	2.443822000	2.743541000	-1.011611000
1	2.150775000	2.306024000	-1.961493000
1	2.434520000	3.824839000	-1.117128000
1	3.452101000	2.421178000	-0.755586000
6	-1.358106000	-1.616067000	-0.013521000
6	-2.382173000	-1.412191000	-0.932278000
6	-1.439176000	-2.688295000	0.868643000
6	-3.469076000	-2.265671000	-0.969567000
6	-2.527487000	-3.539950000	0.828188000
6	-3.543612000	-3.332221000	-0.090204000
1	-2.321903000	-0.580454000	-1.617796000
1	-0.646171000	-2.853177000	1.579683000
1	-4.255749000	-2.098771000	-1.688800000
1	-2.582432000	-4.368085000	1.517686000
1	-4.390434000	-4.000353000	-0.119696000
6	-1.358343000	1.615939000	0.014582000
6	-2.383534000	1.411518000	0.931934000

6	-1.438392000	2.688476000	-0.867370000
6	-3.470726000	2.264661000	0.967963000
6	-2.527036000	3.539773000	-0.828166000
6	-3.544335000	3.331391000	0.088787000
1	-2.323960000	0.579594000	1.617253000
1	-0.644429000	2.853648000	-1.577268000
1	-4.258373000	2.097466000	1.686056000
1	-2.581301000	4.368054000	-1.517530000
1	-4.391377000	3.999292000	0.117336000
6	3.432125000	-0.000550000	-0.001666000
8	3.910203000	-0.694301000	-0.896352000
8	3.915120000	0.692674000	0.890106000
E = -1144.25639899		N _{img} =0	

ImCl₂NⁱPr₂-CO₂

At. No.	x	y	z
6	-0.000069000	0.989204000	0.000090000
7	1.084620000	0.212549000	-0.015567000
7	-1.084653000	0.212464000	0.015844000
6	0.675258000	-1.095907000	-0.011262000
6	-0.675183000	-1.095981000	0.011361000
6	2.467894000	0.731266000	-0.058868000
6	-2.467963000	0.731090000	0.059129000
6	3.170255000	0.307983000	-1.331273000
6	3.205516000	0.379937000	1.214017000
6	-3.170419000	0.307718000	1.331474000
6	-3.205416000	0.379856000	-1.213874000
17	1.690089000	-2.444512000	-0.031101000
17	-1.689819000	-2.444719000	0.030873000
1	2.325706000	1.805040000	-0.066380000
1	2.659648000	0.751072000	2.076331000
1	4.175931000	0.868360000	1.198070000
1	3.370387000	-0.688257000	1.321198000
1	2.574625000	0.556760000	-2.205470000
1	4.107044000	0.853934000	-1.401761000
1	3.402640000	-0.751981000	-1.353697000
1	-2.325866000	1.804870000	0.066850000
1	-3.370001000	-0.688371000	-1.321200000
1	-2.659523000	0.751258000	-2.076058000
1	-4.175947000	0.868046000	-1.197961000
1	-3.402455000	-0.752308000	1.354061000
1	-4.107395000	0.853378000	1.401722000
1	-2.574995000	0.556835000	2.205717000
6	-0.000157000	2.542268000	-0.000108000
8	0.800019000	3.018238000	0.800732000

8 -0.800324000 3.017838000 -0.801181000
E = -1569.64867154 N_{img}=0

Im(NO₂)₂NⁱPr₂-CO₂

At. No.	x	y	z
6	-0.001857000	1.186031000	-0.000065000
7	1.088986000	0.414930000	-0.037618000
7	-1.090574000	0.412125000	0.037622000
6	0.675542000	-0.880290000	-0.019533000
6	-0.673676000	-0.882155000	0.020201000
6	2.466321000	0.963404000	-0.219557000
6	-2.469138000	0.957608000	0.219535000
6	3.207306000	0.213927000	-1.305473000
6	3.187189000	1.046415000	1.105468000
6	-3.208419000	0.207336000	1.306055000
6	-3.190310000	1.038830000	-1.105424000
1	2.272633000	1.975311000	-0.554872000
1	2.615071000	1.660947000	1.792867000
1	4.145252000	1.531997000	0.939720000
1	3.367000000	0.065469000	1.530411000
1	2.600981000	0.102099000	-2.201238000
1	4.080586000	0.800623000	-1.574979000
1	3.562484000	-0.758983000	-0.981760000
1	-2.277509000	1.970067000	0.554383000
1	-3.367579000	0.057498000	-1.530498000
1	-2.619820000	1.654995000	-1.792735000
1	-4.149632000	1.521888000	-0.939550000
1	-3.562600000	-0.766047000	0.982785000
1	-4.082164000	0.793077000	1.576143000
1	-2.601301000	0.096466000	2.201414000
6	-0.003726000	2.744133000	-0.000288000
8	0.855269000	3.208076000	0.740332000
8	-0.863852000	3.205798000	-0.741019000
7	-1.530458000	-2.034860000	0.042721000
8	-1.221557000	-2.912962000	0.806226000
8	-2.471785000	-2.025632000	-0.709617000
7	1.536343000	-2.030216000	-0.042628000
8	1.234330000	-2.906177000	-0.811215000
8	2.473986000	-2.020442000	0.714257000

E = -1059.16549625 N_{img}=0

ImF₂NPh₂-CO₂

At. No.	x	y	z
6	0.000018000	-0.278197000	0.042209000
7	-1.078471000	0.496946000	-0.091722000

7	1.078524000	0.496912000	-0.091748000
6	-0.667887000	1.791686000	-0.306536000
6	0.667979000	1.791665000	-0.306544000
9	1.518723000	2.762084000	-0.501074000
9	-1.518595000	2.762135000	-0.501058000
6	-2.437046000	0.066137000	-0.015623000
6	-2.833112000	-1.039781000	-0.743839000
6	-3.317505000	0.769611000	0.786125000
6	-4.151315000	-1.449658000	-0.653816000
6	-4.634171000	0.355393000	0.852244000
6	-5.050640000	-0.753888000	0.134927000
1	-2.115737000	-1.580385000	-1.341544000
1	-2.975968000	1.621036000	1.353412000
1	-4.471643000	-2.318787000	-1.205816000
1	-5.330852000	0.894155000	1.474520000
1	-6.077382000	-1.078880000	0.196248000
6	2.437089000	0.066078000	-0.015632000
6	3.317557000	0.769592000	0.786065000
6	2.833138000	-1.039888000	-0.743786000
6	4.634219000	0.355360000	0.852208000
6	4.151333000	-1.449784000	-0.653730000
6	5.050670000	-0.753978000	0.134970000
1	2.976038000	1.621071000	1.353284000
1	2.115762000	-1.580512000	-1.341467000
1	5.330909000	0.894160000	1.474441000
1	4.471645000	-2.318954000	-1.205674000
1	6.077408000	-1.078981000	0.196311000
6	-0.000066000	-1.803316000	0.328127000
8	-0.000217000	-2.053429000	1.521986000
8	-0.000192000	-2.462958000	-0.711292000
E = -1074.89466991 N _{img} =0			

ImBicar-CO₂

At. No.	x	y	z
6	-0.000039000	0.843699000	0.000162000
7	1.051096000	0.034606000	-0.048188000
7	-1.051133000	0.034536000	0.048551000
6	0.676777000	-1.283789000	-0.031805000
6	-0.676734000	-1.283853000	0.031601000
6	1.884870000	-2.144736000	-0.120973000
6	2.998847000	-1.151794000	0.251171000
6	2.485182000	0.227792000	-0.160346000
6	-1.884847000	-2.144830000	0.120410000
6	-2.998920000	-1.151695000	-0.250988000
6	-2.485129000	0.227757000	0.161037000

1	-1.851843000	-3.000877000	-0.546185000
1	-2.011332000	-2.521305000	1.135317000
1	-3.150572000	-1.169678000	-1.327639000
1	-3.945301000	-1.391051000	0.222200000
1	-2.799423000	1.049265000	-0.469274000
1	-2.726802000	0.481488000	1.190089000
1	2.011490000	-2.520552000	-1.136115000
1	1.851796000	-3.001199000	0.545074000
1	3.945390000	-1.390910000	-0.221825000
1	3.150193000	-1.170246000	1.327860000
1	2.726899000	0.481992000	-1.189275000
1	2.799420000	1.049123000	0.470246000
6	-0.000002000	2.373226000	-0.000169000
8	1.135862000	2.846726000	-0.041619000
8	-1.135824000	2.846936000	0.041168000
E = -647.979617833 N _{img} =0			

ImCylm-CO₂

At. No.	x	y	z
7	1.074445000	0.240932000	-0.030972000
7	-1.069541000	0.233287000	-0.045584000
6	-0.000453000	1.030219000	-0.022476000
6	2.466757000	0.678875000	0.053515000
6	3.392771000	-0.453860000	-0.322901000
6	3.027842000	-1.731152000	0.407285000
6	1.658891000	-2.197021000	-0.054439000
6	0.685104000	-1.075451000	-0.035360000
6	-0.670391000	-1.080288000	-0.049616000
6	-1.634466000	-2.209367000	-0.089251000
6	-3.013120000	-1.752360000	0.350739000
6	-3.374557000	-0.482871000	-0.394130000
6	-2.467005000	0.662097000	-0.007361000
1	-1.694998000	-2.601813000	-1.106134000
1	-1.263499000	-3.020485000	0.534870000
1	-3.019584000	-1.562718000	1.424641000
1	-3.740375000	-2.537123000	0.158772000
1	-4.397133000	-0.180476000	-0.182707000
1	-3.312590000	-0.662752000	-1.468548000
1	-2.574233000	1.517964000	-0.660005000
1	-2.673722000	1.016825000	0.998223000
1	1.739060000	-2.590168000	-1.069680000
1	1.284375000	-3.010460000	0.564448000
1	3.763139000	-2.509982000	0.221816000
1	3.017600000	-1.548063000	1.482390000
1	3.352956000	-0.624444000	-1.399727000
1	4.408299000	-0.143955000	-0.089497000

1	2.572808000	1.550848000	-0.577094000
1	2.648108000	1.001813000	1.076453000
6	-0.019113000	2.568118000	0.053029000
8	-1.117444000	3.014479000	0.383428000
8	1.060183000	3.091000000	-0.221745000
E = -726.581880495		N _{img} =0	

ImPhen-CO₂

At. No.	x	y	z
7	-1.219834000	0.252404000	-0.069658000
7	0.841615000	0.920602000	-0.078937000
6	-0.431528000	1.333816000	-0.069315000
6	-2.668609000	0.090733000	-0.078364000
6	-3.006077000	-1.255454000	0.552027000
6	-2.281569000	-2.453150000	-0.069965000
6	-0.806366000	-2.197020000	-0.083462000
6	-0.436691000	-0.867819000	-0.086287000
6	0.864794000	-0.445903000	-0.092910000
6	1.944078000	-1.305481000	-0.095990000
6	3.288861000	-0.646736000	-0.092521000
6	3.176962000	0.750834000	0.524951000
6	2.109282000	1.639760000	-0.101811000
1	3.662039000	-0.570006000	-1.115159000
1	4.012659000	-1.240606000	0.460779000
1	4.128497000	1.269421000	0.440759000
1	2.963998000	0.650888000	1.588903000
1	1.976405000	2.576378000	0.423862000
1	2.345556000	1.872968000	-1.138304000
1	-2.515325000	-3.358685000	0.485086000
1	-2.635381000	-2.610175000	-1.090303000
1	-2.765854000	-1.211088000	1.614032000
1	-4.081544000	-1.394070000	0.477056000
1	-3.109722000	0.924855000	0.451020000
1	-3.007243000	0.145472000	-1.110898000
6	1.599208000	-2.645868000	-0.088156000
6	0.259011000	-3.080167000	-0.082464000
1	2.379085000	-3.392824000	-0.076938000
1	0.065729000	-4.142562000	-0.068116000
6	-0.911082000	2.796778000	-0.054785000
8	0.010989000	3.602098000	0.061539000
8	-2.132616000	2.895785000	-0.159950000
E = -801.570681015		N _{img} =0	

IMPhenPh₂-CO₂

At. No.	x	y	z
7	1.007740000	0.520959000	-0.409344000

7	-0.848068000	0.078096000	0.615791000
6	0.238843000	-0.467688000	0.063578000
6	2.329918000	0.484456000	-1.039973000
6	2.899001000	1.914755000	-1.025323000
6	1.960356000	3.047785000	-1.440502000
6	0.710704000	2.981605000	-0.622200000
6	0.368360000	1.715196000	-0.202019000
6	-0.797375000	1.435744000	0.458300000
6	-1.720146000	2.393343000	0.822292000
6	-2.934239000	1.874042000	1.527978000
6	-2.619124000	0.524873000	2.179857000
6	-2.016071000	-0.533142000	1.241585000
1	-3.753350000	1.757565000	0.816600000
1	-3.275015000	2.574911000	2.286809000
1	-3.523586000	0.101196000	2.607543000
1	-1.917083000	0.682920000	2.998347000
1	-1.651853000	-1.375560000	1.819029000
1	2.468980000	4.001187000	-1.317150000
1	1.703837000	2.962476000	-2.497766000
1	3.246035000	2.115772000	-0.012603000
1	3.783672000	1.904353000	-1.656403000
1	2.189327000	0.116584000	-2.054076000
6	-1.372577000	3.682313000	0.452258000
6	-0.193561000	3.967245000	-0.262225000
1	-2.029893000	4.501335000	0.704138000
1	-0.000104000	4.991492000	-0.544628000
6	3.272992000	-0.432470000	-0.307762000
6	3.459081000	-0.293241000	1.059885000
6	3.991732000	-1.393871000	-0.996892000
6	4.359465000	-1.100132000	1.730741000
6	4.903601000	-2.192585000	-0.330484000
6	5.090027000	-2.047227000	1.033279000
1	2.886442000	0.441991000	1.609527000
1	3.804627000	-1.543750000	-2.049222000
1	4.487065000	-0.993119000	2.796847000
1	5.450501000	-2.947215000	-0.874014000
1	5.790871000	-2.681044000	1.554225000
6	-2.992434000	-1.040894000	0.215540000
6	-3.295041000	-0.323730000	-0.933992000
6	-3.636213000	-2.247034000	0.447244000
6	-4.241990000	-0.796431000	-1.825945000
6	-4.586492000	-2.718265000	-0.440851000
6	-4.895120000	-1.991412000	-1.577644000
1	-2.779356000	0.602424000	-1.146674000
1	-3.369993000	-2.831826000	1.315254000
1	-4.464106000	-0.232938000	-2.719157000

1	-5.072044000	-3.663443000	-0.253631000
1	-5.629581000	-2.362023000	-2.275886000
6	0.457722000	-1.979991000	-0.124116000
8	1.030655000	-2.231557000	-1.181807000
8	-0.019608000	-2.655459000	0.785819000
E = -1263.46694325		N _{img} =0	

ImDpylm-CO₂

At. No.	x	y	z
7	-1.073815000	0.150062000	0.000031000
7	1.073889000	0.150996000	0.000026000
6	-0.000238000	0.965845000	0.000033000
6	-2.404207000	0.509770000	0.000039000
6	-3.336426000	-0.465903000	0.000031000
6	-2.977614000	-1.836757000	0.000016000
6	-1.666536000	-2.188097000	0.000009000
6	-0.692672000	-1.178252000	0.000017000
6	0.693716000	-1.177763000	0.000018000
6	1.667968000	-2.187094000	0.000011000
6	2.978943000	-1.835242000	0.000012000
6	3.336860000	-0.464222000	0.000019000
6	2.404170000	0.511049000	0.000025000
1	1.353861000	-3.217854000	0.000006000
1	3.747316000	-2.590602000	0.000007000
1	4.374002000	-0.173648000	0.000017000
1	2.570599000	1.575200000	0.000025000
1	-1.352119000	-3.218750000	-0.000001000
1	-3.745593000	-2.592536000	0.000012000
1	-4.373809000	-0.176201000	0.000039000
1	-2.570398000	1.573985000	0.000057000
6	-0.001068000	2.496032000	0.000045000
8	1.127788000	2.989281000	-0.000014000
8	-1.130506000	2.987819000	-0.000262000
E = -721.732028230		N _{img} =0	

BImNMe₂-CO₂

At. No.	x	y	z
7	-0.321712000	-1.083361000	-0.045069000
7	-0.321704000	1.083384000	0.044962000
6	-1.099428000	0.000011000	-0.000041000
6	-0.751807000	-2.463392000	-0.123044000
6	0.998487000	-0.692591000	-0.034069000
6	0.998497000	0.692600000	0.034040000
6	-0.751839000	2.463400000	0.123082000
1	-1.827010000	-2.486809000	-0.005025000
1	-1.826931000	2.486871000	0.004061000

1	-0.450874000	-2.880717000	-1.079397000
1	-0.287229000	-3.021610000	0.683905000
1	-0.451841000	2.880359000	1.079888000
1	-0.286455000	3.021918000	-0.683194000
6	2.175525000	1.419875000	0.075712000
1	2.174953000	2.496314000	0.133119000
6	2.175517000	-1.419867000	-0.075715000
1	2.174969000	-2.496307000	-0.133125000
6	3.351008000	0.697577000	0.037615000
6	3.351000000	-0.697572000	-0.037579000
1	4.292998000	1.221595000	0.065460000
1	4.292982000	-1.221605000	-0.065392000
6	-2.651626000	-0.000004000	0.000012000
8	-3.129653000	0.962847000	-0.593534000
8	-3.129554000	-0.962896000	0.593580000
E =	-646.776126060	N _{img} =0	

BImNEt₂-CO₂

At. No.	x	y	z
7	-0.114577000	1.074358000	-0.282712000
7	-0.242869000	-1.093210000	-0.227965000
6	-0.950551000	0.035257000	-0.287932000
6	-0.471929000	2.486244000	-0.345486000
6	1.177816000	0.608394000	-0.196494000
6	1.095570000	-0.777289000	-0.151183000
6	-0.778118000	-2.449263000	-0.185374000
1	-1.446074000	2.552254000	-0.811209000
1	-1.627239000	-2.471182000	-0.856583000
1	0.264264000	2.959038000	-0.991556000
1	0.004055000	-3.095802000	-0.572315000
6	2.228991000	-1.567870000	-0.048597000
1	2.170849000	-2.643203000	-0.005110000
6	2.396797000	1.266075000	-0.153381000
1	2.461461000	2.341763000	-0.186305000
6	3.442555000	-0.914381000	-0.002336000
6	3.525553000	0.479440000	-0.055036000
1	4.349618000	-1.491889000	0.078010000
1	4.494584000	0.950573000	-0.013302000
6	-0.507772000	3.111870000	1.028130000
1	0.443362000	3.006105000	1.545617000
1	-0.730441000	4.171790000	0.939535000
1	-1.294916000	2.643133000	1.609883000
6	-1.186493000	-2.842700000	1.214624000
1	-1.523588000	-3.875603000	1.219780000
1	-0.360021000	-2.748025000	1.915297000
1	-2.010884000	-2.220840000	1.552002000

6	-2.494497000	0.132669000	-0.308917000
8	-3.040656000	-0.825462000	-0.848469000
8	-2.904399000	1.155860000	0.236329000
E = -725.369418601		N _{img} =0	

Py[b]ImNMe₂-CO₂

At. No.	x	y	z
7	0.302595000	-1.060631000	-0.050577000
7	0.307128000	1.114651000	0.035191000
6	1.078808000	0.023504000	-0.008711000
6	0.724255000	-2.449733000	-0.093792000
6	-1.012885000	-0.661712000	-0.032912000
6	-1.009015000	0.725799000	0.029640000
6	0.747634000	2.493671000	0.104249000
1	1.170875000	-2.723884000	0.852776000
1	1.821755000	2.503748000	-0.031862000
1	-0.164436000	-3.035164000	-0.295318000
1	1.464952000	-2.582480000	-0.870541000
1	0.268062000	3.054327000	-0.692099000
1	0.471420000	2.911630000	1.067652000
6	-2.211470000	1.403301000	0.066438000
1	-2.270856000	2.478814000	0.118023000
7	-2.073595000	-1.434112000	-0.070430000
6	-3.340352000	0.607363000	0.030928000
6	-3.224946000	-0.781979000	-0.037413000
1	-4.321370000	1.052387000	0.054144000
1	-4.115306000	-1.391802000	-0.066267000
6	2.629586000	-0.019642000	0.002231000
8	3.049295000	-1.075362000	0.463859000
8	3.154745000	0.994065000	-0.451326000
E = -662.811063113		N _{img} =0	

Py[c]ImNMe₂-CO₂

At. No.	x	y	z
7	0.314458000	-1.081519000	0.045957000
7	0.310287000	1.089217000	-0.049905000
6	1.088780000	0.000747000	-0.002838000
6	0.747820000	-2.462379000	0.124494000
6	-1.003952000	-0.685591000	0.035442000
6	-1.004582000	0.697446000	-0.036175000
6	0.747418000	2.468379000	-0.130929000
1	1.819777000	-2.484756000	-0.020553000
1	1.818744000	2.487979000	0.019937000
1	0.472562000	-2.871462000	1.091678000
1	0.262272000	-3.025844000	-0.665770000
1	0.479443000	2.875836000	-1.100917000

1	0.260394000	3.036052000	0.655442000
6	-2.199358000	1.391531000	-0.077385000
1	-2.254614000	2.465692000	-0.138176000
6	-2.202163000	-1.377410000	0.078053000
1	-2.243096000	-2.455158000	0.139348000
6	-3.336866000	0.608274000	-0.032821000
7	-3.345617000	-0.723887000	0.042548000
1	-4.308305000	1.078301000	-0.058609000
6	2.642835000	0.002398000	0.001033000
8	3.112565000	0.949626000	0.623981000
8	3.119851000	-0.943836000	-0.617210000
E = -662.803192348		N _{img} =0	

ImBicar-i

At. No.	x	y	z
6	0.000048000	1.411208000	0.460019000
7	-1.024720000	0.560395000	0.273821000
7	1.024840000	0.560466000	0.273469000
6	-0.673555000	-0.741766000	-0.016859000
6	0.673633000	-0.741673000	-0.017252000
6	-1.900372000	-1.555998000	-0.195439000
6	-2.989803000	-0.483171000	-0.388716000
6	-2.448994000	0.782700000	0.283127000
6	1.900369000	-1.555874000	-0.196396000
6	2.989897000	-0.483077000	-0.389320000
6	2.449086000	0.782907000	0.282331000
1	2.793530000	0.869179000	1.317600000
1	-2.793126000	0.868492000	1.318546000
1	-2.108438000	-2.154093000	0.693461000
1	2.108497000	-2.154439000	0.692165000
8	-2.794949000	1.917726000	-0.433695000
8	2.794837000	1.917627000	-0.435099000
1	2.183813000	2.614677000	-0.186531000
1	-2.183297000	2.614413000	-0.185617000
1	-3.042089000	-0.232404000	-1.449012000
1	-1.851244000	-2.237122000	-1.040345000
1	1.851034000	-2.236587000	-1.041629000
1	3.042671000	-0.232309000	-1.449586000
6	-4.356600000	-0.913540000	0.099423000
1	-4.618893000	-1.856779000	-0.383709000
1	-4.298638000	-1.128446000	1.169874000
6	4.356480000	-0.913588000	0.099287000

1	4.618745000	-1.856903000	-0.383716000
1	4.298194000	-1.128390000	1.169742000
6	5.455185000	0.101045000	-0.155274000
1	5.208708000	1.040515000	0.337989000
1	5.491197000	0.328831000	-1.220971000
6	-5.455114000	0.101289000	-0.155333000
1	-5.490408000	0.329693000	-1.220914000
1	-5.208926000	1.040456000	0.338636000
6	-6.810453000	-0.387982000	0.313029000
1	-7.587006000	0.348708000	0.122410000
1	-7.094308000	-1.307521000	-0.196513000
1	-6.806018000	-0.593702000	1.382364000
6	6.810164000	-0.387960000	0.314346000
1	7.094207000	-1.308054000	-0.194092000
1	7.586934000	0.348426000	0.123445000
1	6.805092000	-0.592613000	1.383889000
E = -845.599142332 N _{img} =0			

ImBicar-ii

At. No.	x	y	z
6	-0.177121000	1.646265000	0.583137000
7	-1.208563000	0.961466000	0.045316000
7	0.816191000	0.779205000	0.323091000
6	-0.877030000	-0.251342000	-0.532133000
6	0.450381000	-0.369438000	-0.344899000
6	-2.083652000	-0.876618000	-1.122701000
6	-3.237673000	-0.038160000	-0.507109000
6	-2.595415000	1.298912000	-0.123160000
6	1.643914000	-1.223625000	-0.549286000
6	2.801906000	-0.236786000	-0.305941000
6	2.224835000	0.853790000	0.606974000
1	2.405688000	0.605727000	1.655794000
1	-3.003809000	1.692580000	0.805584000
7	3.964506000	-0.875613000	0.257038000
7	-3.904776000	-0.643480000	0.623446000
6	4.452896000	-1.928988000	-0.598029000
1	5.323412000	-2.388946000	-0.138385000
1	3.700991000	-2.701973000	-0.727776000
1	4.746565000	-1.561476000	-1.592056000
6	5.020969000	0.074544000	0.522196000
1	5.859071000	-0.444584000	0.979480000
1	5.374758000	0.571048000	-0.391259000
1	4.682342000	0.845471000	1.206123000
6	-4.756664000	-1.734778000	0.232648000
1	-5.345233000	-2.057341000	1.088047000
1	-5.442589000	-1.408626000	-0.545338000

1	-4.205654000	-2.610088000	-0.140021000
6	-3.030552000	-1.021899000	1.706314000
1	-3.633960000	-1.370939000	2.540355000
1	-2.330304000	-1.824508000	1.438267000
1	-2.450387000	-0.169399000	2.047800000
1	-2.187159000	-1.932563000	-0.881864000
1	1.693459000	-2.020630000	0.193788000
8	-2.779688000	2.190173000	-1.178502000
8	2.732195000	2.106877000	0.300013000
1	2.092497000	2.755520000	0.603861000
1	-2.237419000	2.962104000	-1.016242000
1	-3.999358000	0.170555000	-1.252393000
1	-2.082725000	-0.785441000	-2.207177000
1	1.686711000	-1.676007000	-1.535433000
1	3.040778000	0.270795000	-1.253548000
E = -877.628869547 N _{img} =0			

ImN(CH₂OH)₂

At. No.	x	y	z
6	-0.001770000	-0.663988000	-0.651018000
7	1.050004000	0.121145000	-0.327043000
7	-1.051483000	0.124441000	-0.327890000
6	0.672018000	1.340481000	0.195864000
6	-0.670069000	1.342435000	0.195564000
6	2.411123000	-0.320802000	-0.456226000
6	-2.413402000	-0.315509000	-0.454581000
1	-3.016203000	0.483173000	-0.874465000
1	3.012763000	0.473619000	-0.885842000
1	2.386956000	-1.172593000	-1.130153000
1	-2.393122000	-1.161464000	-1.135913000
1	-1.374127000	2.084826000	0.517889000
1	1.378241000	2.080788000	0.518214000
8	-2.988048000	-0.630029000	0.770559000
1	-2.533092000	-1.387257000	1.136574000
8	2.991055000	-0.624663000	0.769027000
1	2.537475000	-1.378362000	1.143918000
E = -455.049160239 N _{img} =0			

ImN(CH₂NHCOMe)₂

At. No.	x	y	z
6	0.000074000	-1.311778000	0.000328000
7	0.932696000	-0.460193000	-0.479303000
7	-0.932479000	-0.459668000	0.479159000
6	0.599468000	0.868482000	-0.304398000
6	-0.599111000	0.868835000	0.303077000
1	-1.246104000	1.668185000	0.611582000

1	1.246494000	1.667508000	-0.613687000
6	2.174829000	-0.913976000	-1.044754000
7	3.277313000	-0.818694000	-0.136639000
1	3.374163000	-1.526013000	0.565607000
6	4.001298000	0.322775000	-0.032575000
8	3.802892000	1.276342000	-0.758191000
1	2.028537000	-1.948064000	-1.330273000
1	2.417104000	-0.313632000	-1.914889000
6	5.061991000	0.336863000	1.027031000
1	5.231115000	-0.633994000	1.482369000
1	5.985772000	0.695691000	0.585861000
1	4.769415000	1.044455000	1.797936000
6	-2.174529000	-0.912982000	1.045182000
7	-3.277168000	-0.818453000	0.137182000
1	-3.374238000	-1.526459000	-0.564337000
6	-4.001287000	0.322839000	0.032461000
8	-3.802547000	1.277086000	0.757098000
1	-2.028135000	-1.946841000	1.331477000
1	-2.416648000	-0.311972000	1.914902000
6	-5.063028000	0.335748000	-1.026116000
1	-5.227656000	-0.634061000	-1.485311000
1	-5.988290000	0.687780000	-0.582490000
1	-4.775064000	1.048216000	-1.794204000
E = -720.529429937 N _{img} =0			

ImN(CH₂NHPh)₂

At. No.	x	y	z
6	-0.283650000	0.252914000	-0.287282000
7	-1.089854000	1.325590000	-0.157342000
7	0.918722000	0.828003000	-0.507732000
6	-0.420159000	2.520802000	-0.281952000
6	0.866700000	2.204342000	-0.504794000
1	1.732027000	2.819664000	-0.655353000
1	-0.906251000	3.474847000	-0.211967000
6	-2.495224000	1.221855000	0.156039000
7	-3.017834000	0.035232000	-0.434977000
1	-2.312266000	-0.680496000	-0.516255000
1	-2.625616000	1.233379000	1.244228000
1	-2.991638000	2.103825000	-0.248134000
6	2.117536000	0.073677000	-0.739408000
7	3.052336000	0.320402000	0.318400000
1	2.628877000	0.269692000	1.228422000
1	1.811990000	-0.969065000	-0.830060000
1	2.563401000	0.390446000	-1.680010000
6	-4.290381000	-0.382556000	-0.112417000
6	-5.220996000	0.474817000	0.472289000

6	-4.683237000	-1.690740000	-0.405826000
6	-6.505148000	0.033383000	0.745451000
6	-5.962837000	-2.118268000	-0.124989000
6	-6.889438000	-1.261185000	0.452718000
1	-4.951769000	1.491523000	0.712344000
1	-3.971884000	-2.364132000	-0.861141000
1	-7.208861000	0.716583000	1.196760000
1	-6.241159000	-3.134616000	-0.359855000
1	-7.889685000	-1.600393000	0.669923000
6	4.332440000	-0.208615000	0.260593000
6	4.853494000	-0.783364000	-0.895658000
6	5.146586000	-0.135123000	1.392564000
6	6.158617000	-1.248655000	-0.916833000
6	6.439154000	-0.612461000	1.362286000
6	6.962026000	-1.169713000	0.204165000
1	4.248450000	-0.883186000	-1.782052000
1	4.754808000	0.312210000	2.294777000
1	6.541381000	-1.688482000	-1.825318000
1	7.046958000	-0.543879000	2.251749000
1	7.974749000	-1.539179000	0.181809000
E = -877.212578585 N _{img} =0			

ImBicar-iii

At. No.	x	y	z
6	-0.000010000	0.000051000	1.665983000
7	-0.676012000	0.776816000	0.793664000
7	0.676022000	-0.776780000	0.793736000
6	-0.448395000	0.501760000	-0.540875000
6	0.448448000	-0.501816000	-0.540830000
6	-1.292963000	1.372373000	-1.395475000
6	-1.785624000	2.421276000	-0.383926000
6	-1.711511000	1.773648000	1.002738000
6	1.293071000	-1.372469000	-1.395339000
6	1.785760000	-2.421273000	-0.383701000
6	1.711538000	-1.773574000	1.002915000
1	0.747415000	-1.826474000	-2.218028000
1	2.126046000	-0.810458000	-1.815391000
1	1.114036000	-3.275891000	-0.395481000
1	2.786000000	-2.781813000	-0.597188000
1	-2.125950000	0.810379000	-1.815517000
1	-0.747250000	1.826289000	-2.218178000
1	-2.785813000	2.781918000	-0.597470000
1	-1.113813000	3.275824000	-0.395725000
1	-1.379260000	2.473610000	1.762429000
7	-2.963879000	1.221550000	1.470210000
1	-2.793114000	0.802790000	2.372167000

6	-3.587395000	0.279208000	0.609159000
6	-4.587243000	0.711194000	-0.251870000
6	-3.220606000	-1.061659000	0.603670000
6	-5.194070000	-0.176542000	-1.123086000
6	-3.841632000	-1.952094000	-0.255205000
6	-4.822608000	-1.511292000	-1.127776000
1	-4.890714000	1.746270000	-0.213521000
1	-2.437198000	-1.393443000	1.270628000
1	-5.970230000	0.171140000	-1.787806000
1	-3.552109000	-2.992002000	-0.247812000
1	-5.302545000	-2.205254000	-1.800547000
1	1.379293000	-2.473521000	1.762624000
7	2.963874000	-1.221382000	1.470405000
1	2.793023000	-0.802490000	2.372287000
6	3.587386000	-0.279148000	0.609244000
6	4.586949000	-0.711295000	-0.252034000
6	3.220837000	1.061785000	0.603867000
6	5.193718000	0.176353000	-1.123374000
6	3.841812000	1.952132000	-0.255136000
6	4.822498000	1.511173000	-1.127952000
1	4.890241000	-1.746431000	-0.213792000
1	2.437633000	1.393695000	1.271001000
1	5.969658000	-0.171460000	-1.788283000
1	3.552458000	2.992088000	-0.247665000
1	5.302404000	2.205060000	-1.800822000
E = -1031.99778689 N _{img} =0			

ImBicar-i-CO₂

At. No.	x	y	z
6	0.000004000	1.000819000	-0.107043000
7	1.053235000	0.197308000	-0.029083000
7	-1.053224000	0.197273000	-0.029316000
6	0.679363000	-1.110743000	0.081865000
6	-0.679355000	-1.110762000	0.081730000
6	1.886615000	-1.973021000	0.114052000
6	3.017592000	-0.967672000	0.397225000
6	2.509220000	0.407622000	-0.048842000
6	-1.886616000	-1.973027000	0.113912000
6	-3.017569000	-0.967643000	0.397072000
6	-2.509194000	0.407599000	-0.049171000
1	-2.779565000	0.636934000	-1.083573000
1	2.779615000	0.637139000	-1.083193000
1	2.035067000	-2.459295000	-0.850926000
1	-2.035094000	-2.459299000	-0.851062000

8	2.906988000	1.385777000	0.812423000
8	-2.906917000	1.385947000	0.811895000
1	-2.481966000	2.208864000	0.503071000
1	2.482512000	2.208865000	0.503624000
1	3.138386000	-0.875846000	1.477126000
1	1.834563000	-2.753001000	0.867721000
1	-1.834601000	-2.752997000	0.867591000
1	-3.138328000	-0.875709000	1.476965000
6	4.340657000	-1.355891000	-0.229948000
1	4.605598000	-2.359540000	0.107614000
1	4.212148000	-1.424828000	-1.313508000
6	-4.340673000	-1.355877000	-0.229984000
1	-4.605498000	-2.359581000	0.107530000
1	-4.212263000	-1.424700000	-1.313558000
6	-5.477132000	-0.402046000	0.087542000
1	-5.216823000	0.601885000	-0.245738000
1	-5.591195000	-0.330068000	1.169319000
6	5.477105000	-0.401984000	0.087377000
1	5.591321000	-0.329922000	1.169122000
1	5.216720000	0.601913000	-0.245922000
6	6.783711000	-0.836338000	-0.543967000
1	7.587264000	-0.144349000	-0.305560000
1	7.082434000	-1.823358000	-0.194227000
1	6.700300000	-0.883270000	-1.628622000
6	-6.783817000	-0.836334000	-0.543643000
1	-7.082141000	-1.823686000	-0.194499000
1	-7.587508000	-0.144766000	-0.304543000
1	-6.700677000	-0.882500000	-1.628369000
6	-0.000004000	2.506191000	-0.279335000
8	1.128324000	3.005603000	-0.347987000
8	-1.128367000	3.005634000	-0.347661000
E = -1034.16102264		N _{img} =0	

ImBicar-ii-CO₂

At. No.	x	y	z
6	0.004535000	1.222426000	0.119825000
7	-1.072090000	0.452744000	0.025399000
7	1.032144000	0.383589000	0.083280000
6	-0.738483000	-0.869640000	-0.061277000
6	0.618837000	-0.911507000	-0.023669000
6	-1.962477000	-1.700771000	-0.125072000
6	-3.063779000	-0.649936000	-0.436891000
6	-2.512778000	0.726742000	-0.029222000
6	1.794078000	-1.814109000	-0.018119000
6	2.962765000	-0.849860000	-0.292546000
6	2.489677000	0.546845000	0.138603000

1	2.752993000	0.749175000	1.179128000
1	-2.824478000	1.033503000	0.968881000
6	0.041622000	2.730855000	0.266050000
8	-1.074671000	3.257510000	0.296850000
8	1.181442000	3.202034000	0.352654000
7	4.167227000	-1.252902000	0.386944000
7	-4.376755000	-0.889530000	0.086668000
6	4.589290000	-2.565924000	-0.037531000
1	5.493283000	-2.840958000	0.498031000
1	3.832353000	-3.310740000	0.192043000
1	4.803801000	-2.610337000	-1.114661000
6	5.242094000	-0.303172000	0.192366000
1	6.116659000	-0.647572000	0.736852000
1	5.509767000	-0.185979000	-0.865021000
1	4.968789000	0.674713000	0.573090000
6	-5.138200000	-1.828574000	-0.693782000
1	-6.166527000	-1.841204000	-0.341243000
1	-5.145987000	-1.523414000	-1.736605000
1	-4.752629000	-2.856123000	-0.633059000
6	-4.449405000	-1.187202000	1.492473000
1	-5.477833000	-1.077442000	1.827157000
1	-4.128675000	-2.207835000	1.740667000
1	-3.843987000	-0.493601000	2.069664000
1	-2.144852000	-2.186733000	0.832336000
1	1.928307000	-2.270179000	0.962932000
8	-2.826165000	1.661032000	-0.969542000
8	2.932633000	1.511316000	-0.715639000
1	2.511629000	2.345269000	-0.425916000
1	-2.428226000	2.495274000	-0.664402000
1	-3.159407000	-0.576656000	-1.518608000
1	-1.910511000	-2.476451000	-0.882999000
1	1.722358000	-2.606732000	-0.756173000
1	3.116920000	-0.775458000	-1.379959000
E = -1066.18599994 N _{img} =0			

ImN(CH₂OH)₂-CO₂

At. No.	x	y	z
6	0.000398000	0.023004000	-0.211251000
7	1.073390000	0.811782000	-0.164459000
7	-1.074800000	0.809055000	-0.167181000
6	0.672957000	2.112027000	-0.074104000
6	-0.677897000	2.110318000	-0.075917000
6	2.483201000	0.365685000	-0.201506000
6	-2.483194000	0.359156000	-0.205692000
1	-3.072343000	1.269103000	-0.246352000
1	3.069943000	1.277546000	-0.233416000

6	0.002124000	-1.505113000	-0.271964000
8	1.129234000	-2.004141000	-0.297386000
8	-1.123858000	-2.006850000	-0.287953000
1	2.603286000	-0.197035000	-1.122582000
1	-2.598659000	-0.211052000	-1.122708000
1	-1.381235000	2.917014000	-0.013167000
1	1.374047000	2.920524000	-0.009423000
8	-2.830952000	-0.347807000	0.902738000
1	-2.440246000	-1.226172000	0.779488000
8	2.829230000	-0.348616000	0.902618000
1	2.440318000	-1.226918000	0.772098000
E = -643.600574714		N _{img} =0	

ImN(CH₂NHCOMe)₂-CO₂

At. No.	x	y	z
6	0.000028000	0.352965000	0.000199000
7	0.884274000	-0.438165000	0.604030000
7	-0.883939000	-0.438508000	-0.603585000
6	0.560813000	-1.746978000	0.376660000
6	-0.559921000	-1.747201000	-0.376232000
1	-1.169603000	-2.546480000	-0.748672000
1	1.170956000	-2.545965000	0.748991000
6	2.042802000	0.012504000	1.378555000
7	3.096052000	0.466954000	0.550762000
1	3.000177000	1.414334000	0.223627000
6	3.880508000	-0.441145000	-0.080935000
8	3.752804000	-1.633665000	0.123008000
1	1.720955000	0.815905000	2.025300000
1	2.375354000	-0.844920000	1.950753000
6	-0.000064000	1.884093000	-0.000133000
8	-1.079732000	2.378744000	-0.331648000
8	1.079606000	2.378966000	0.331102000
6	4.920591000	0.111361000	-1.004483000
1	4.805626000	1.174594000	-1.187399000
1	5.898389000	-0.067136000	-0.565474000
1	4.878427000	-0.430613000	-1.943263000
6	-2.042562000	0.011712000	-1.378292000
7	-3.095824000	0.466526000	-0.550751000
1	-2.999986000	1.414043000	-0.224014000
6	-3.880850000	-0.441166000	0.080831000
8	-3.753600000	-1.633770000	-0.122862000
1	-1.720746000	0.814807000	-2.025446000
1	-2.375084000	-0.846033000	-1.950026000
6	-4.920940000	0.111952000	1.004009000
1	-4.806185000	1.175373000	1.185953000
1	-5.898753000	-0.067203000	0.565312000

1 -4.878521000 -0.429134000 1.943295000
E = -909.080963837 N_{img}=0

ImN(CH₂NHPh)₂-CO₂

At. No.	x	y	z
6	0.000469000	0.599963000	0.000663000
7	-0.710658000	-0.191944000	-0.804261000
7	0.710956000	-0.190557000	0.807509000
6	-0.448506000	-1.495864000	-0.501558000
6	0.447773000	-1.494982000	0.507958000
1	0.912771000	-2.305493000	1.033008000
1	-0.914320000	-2.307275000	-1.024483000
6	-1.675790000	0.248420000	-1.842130000
7	-2.852655000	0.817383000	-1.325064000
1	-2.672526000	1.756225000	-1.002481000
1	-1.171302000	0.984940000	-2.451417000
1	-1.875858000	-0.638049000	-2.435026000
6	0.000702000	2.135246000	-0.000899000
8	0.839993000	2.632250000	0.751463000
8	-0.838495000	2.630952000	-0.754194000
6	1.677357000	0.251624000	1.843512000
7	2.853812000	0.818970000	1.323893000
1	2.674118000	1.757610000	1.000524000
1	1.173857000	0.989803000	2.451627000
1	1.877610000	-0.633710000	2.438067000
6	-3.756287000	0.086633000	-0.568610000
6	-3.929743000	-1.286742000	-0.721557000
6	-4.556619000	0.757508000	0.354984000
6	-4.878891000	-1.961298000	0.027506000
6	-5.500976000	0.076222000	1.095154000
6	-5.670861000	-1.291069000	0.941337000
1	-3.346629000	-1.838154000	-1.442895000
1	-4.430647000	1.822611000	0.483087000
1	-4.999529000	-3.024808000	-0.113776000
1	-6.108355000	0.620333000	1.802278000
1	-6.408149000	-1.821790000	1.522130000
6	3.756377000	0.086834000	0.567614000
6	3.928311000	-1.286712000	0.720745000
6	4.557251000	0.756623000	-0.356319000
6	4.876545000	-1.962464000	-0.028453000
6	5.500560000	0.074131000	-1.096670000
6	5.668972000	-1.293334000	-0.942655000
1	3.344705000	-1.837413000	1.442215000
1	4.432461000	1.821844000	-0.484588000
1	4.995940000	-3.026095000	0.112983000
1	6.108334000	0.617405000	-1.804098000

1 6.405486000 -1.824981000 -1.523580000
E = -1065.76590397 N_{img}=0

ImBicar-iii-CO₂

At. No.	x	y	z
6	0.037245000	-0.127608000	0.924665000
7	0.609827000	-0.952182000	0.054506000
7	-0.557861000	0.800638000	0.185293000
6	0.390131000	-0.548764000	-1.231490000
6	-0.371811000	0.571534000	-1.147522000
6	1.087938000	-1.447109000	-2.184421000
6	1.575274000	-2.581945000	-1.266218000
6	1.556150000	-2.072893000	0.183514000
6	-1.077075000	1.600563000	-1.951519000
6	-1.461749000	2.635543000	-0.881157000
6	-1.441778000	1.939977000	0.488150000
1	-0.444948000	2.031495000	-2.722527000
1	-1.951502000	1.172697000	-2.436937000
1	-0.717984000	3.427333000	-0.867590000
1	-2.426280000	3.095493000	-1.058930000
1	1.913369000	-0.927405000	-2.665305000
1	0.429138000	-1.816165000	-2.965420000
1	2.562973000	-2.945008000	-1.524759000
1	0.889611000	-3.421384000	-1.339500000
1	1.129031000	-2.798495000	0.864693000
6	0.061569000	-0.218196000	2.438506000
8	0.859053000	-1.056701000	2.870691000
8	-0.718511000	0.564928000	2.989954000
7	2.809471000	-1.674716000	0.747601000
1	2.645861000	-1.574449000	1.740704000
6	3.399235000	-0.495156000	0.240940000
6	4.102940000	-0.502624000	-0.956704000
6	3.303215000	0.691479000	0.960797000
6	4.675773000	0.662005000	-1.437532000
6	3.896037000	1.848715000	0.487273000
6	4.575322000	1.842373000	-0.719185000
1	4.229211000	-1.432261000	-1.490103000
1	2.765844000	0.690000000	1.899404000
1	5.226106000	0.640273000	-2.366057000
1	3.822475000	2.758473000	1.063561000
1	5.036667000	2.744562000	-1.089667000
1	-0.957791000	2.543158000	1.246418000
7	-2.701663000	1.539712000	1.032415000
1	-2.517037000	1.267183000	1.989158000
6	-3.402066000	0.513451000	0.359667000
6	-4.159900000	0.794961000	-0.770740000

6	-3.367106000	-0.791202000	0.840818000
6	-4.843274000	-0.214969000	-1.424571000
6	-4.071056000	-1.794411000	0.197359000
6	-4.802302000	-1.513710000	-0.944352000
1	-4.238690000	1.815273000	-1.112941000
1	-2.790201000	-1.006321000	1.729818000
1	-5.432602000	0.019540000	-2.298174000
1	-4.043249000	-2.799658000	0.589560000
1	-5.349032000	-2.296390000	-1.446931000
E = -1220.55277145		N _{img} =0	
