

Electronic Supplementary Information

Valence tautomeric dinuclear adducts of Co(II) diketonates with redox-active diquinones for the design of spin qubits: computational modeling

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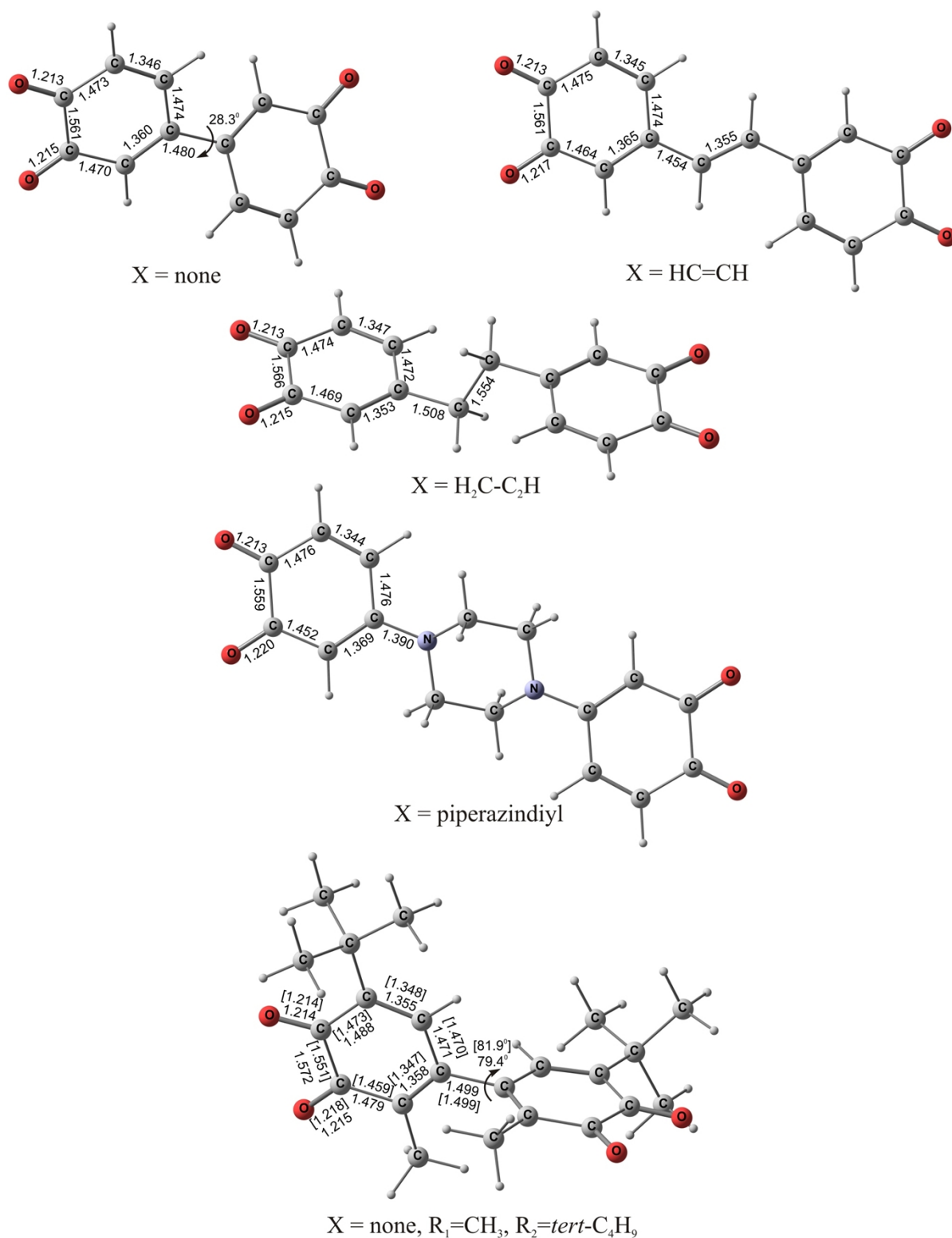


Figure S1. Optimized geometries of the structures of the ligands calculated by the B3LYP*/6-311++G(d,p) method. Hereinafter bond lengths are given in Å, angles are given in degrees. Figures in brackets are the X-ray determined parameters.^{15a}

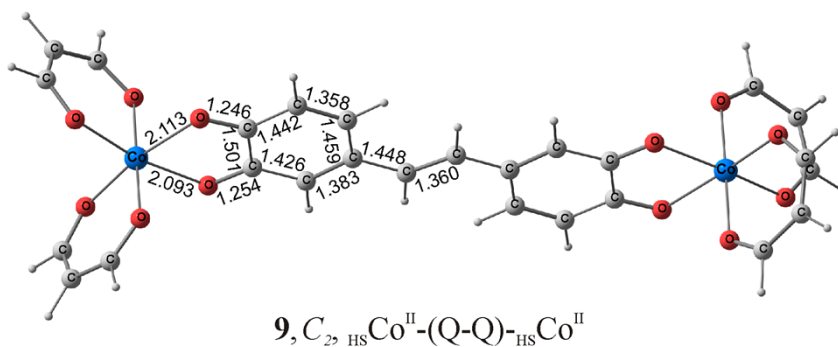
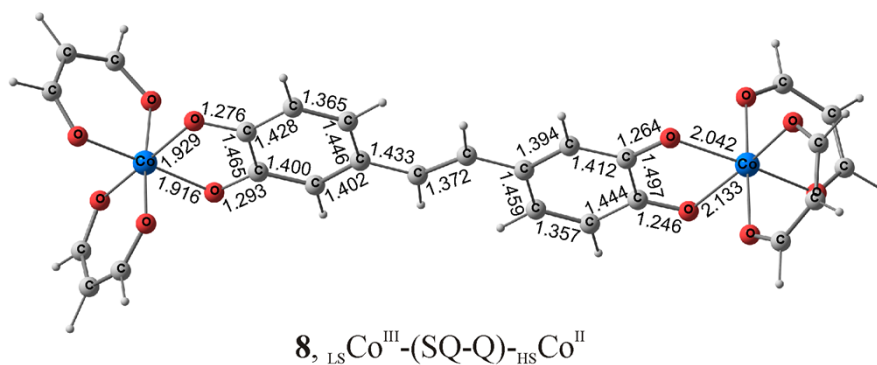
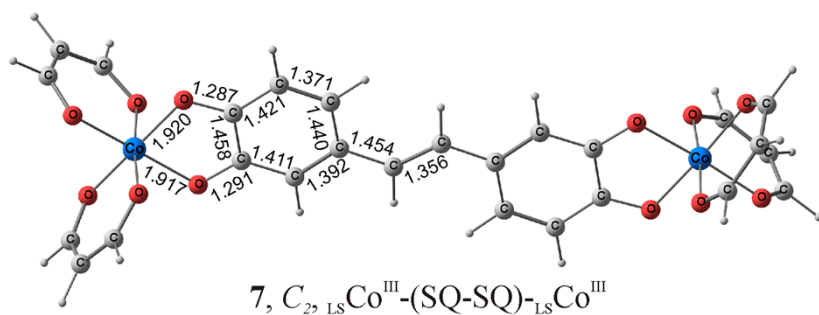
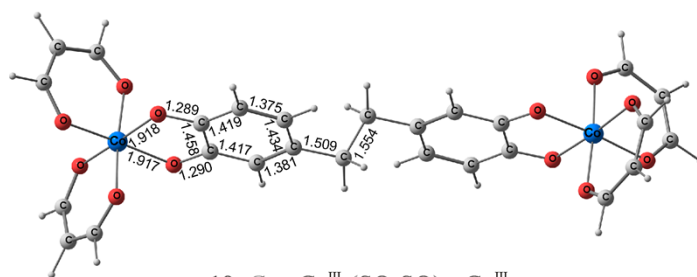
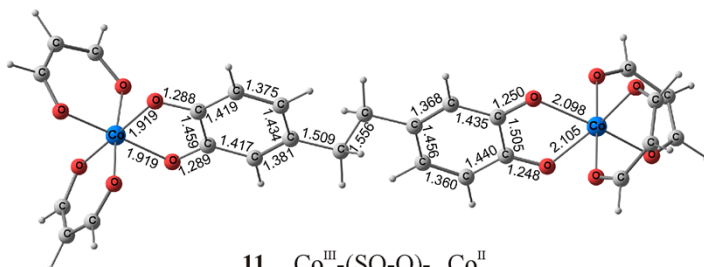


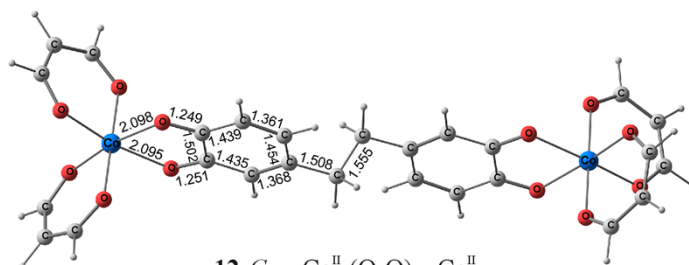
Fig. S2 Optimized geometries of the isomeric structures **7-9** of adduct **1** ($R=H$; $R_1=R_2=H$; $HC=CH$) calculated by the B3LYP*/6-311++G(d,p) method.



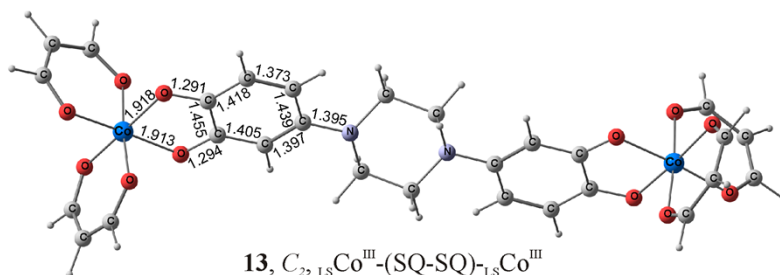
10, C_{2v} , $LS\ Co^{III}-(SQ-SQ)-_{LS}\ Co^{III}$



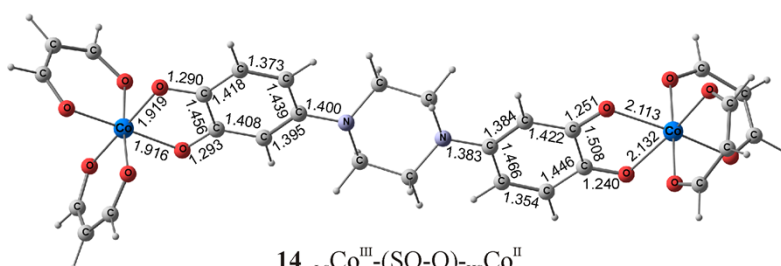
11, $_{LS}\ Co^{III}-(SQ-Q)-_{HS}\ Co^{II}$



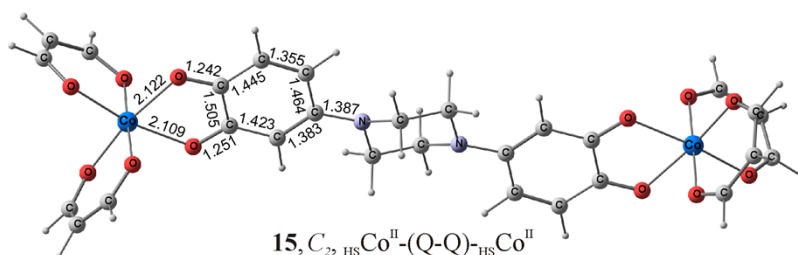
12, C_{2v} , $_{HS}\ Co^{II}-(Q-Q)-_{HS}\ Co^{II}$



13, C_{2v} , $_{LS}\ Co^{III}-(SQ-SQ)-_{LS}\ Co^{III}$



14, $_{LS}\ Co^{III}-(SQ-Q)-_{HS}\ Co^{II}$



15, C_{2v} , $_{HS}\ Co^{II}-(Q-Q)-_{HS}\ Co^{II}$

Fig. S3 Optimized geometries of the structures **10-15** of adducts **1** ($R=H$; $R_1=R_2=H$; $X=H_2C-CH_2$, piperazindyl) calculated by the B3LYP*/6-311++G(d,p) method.

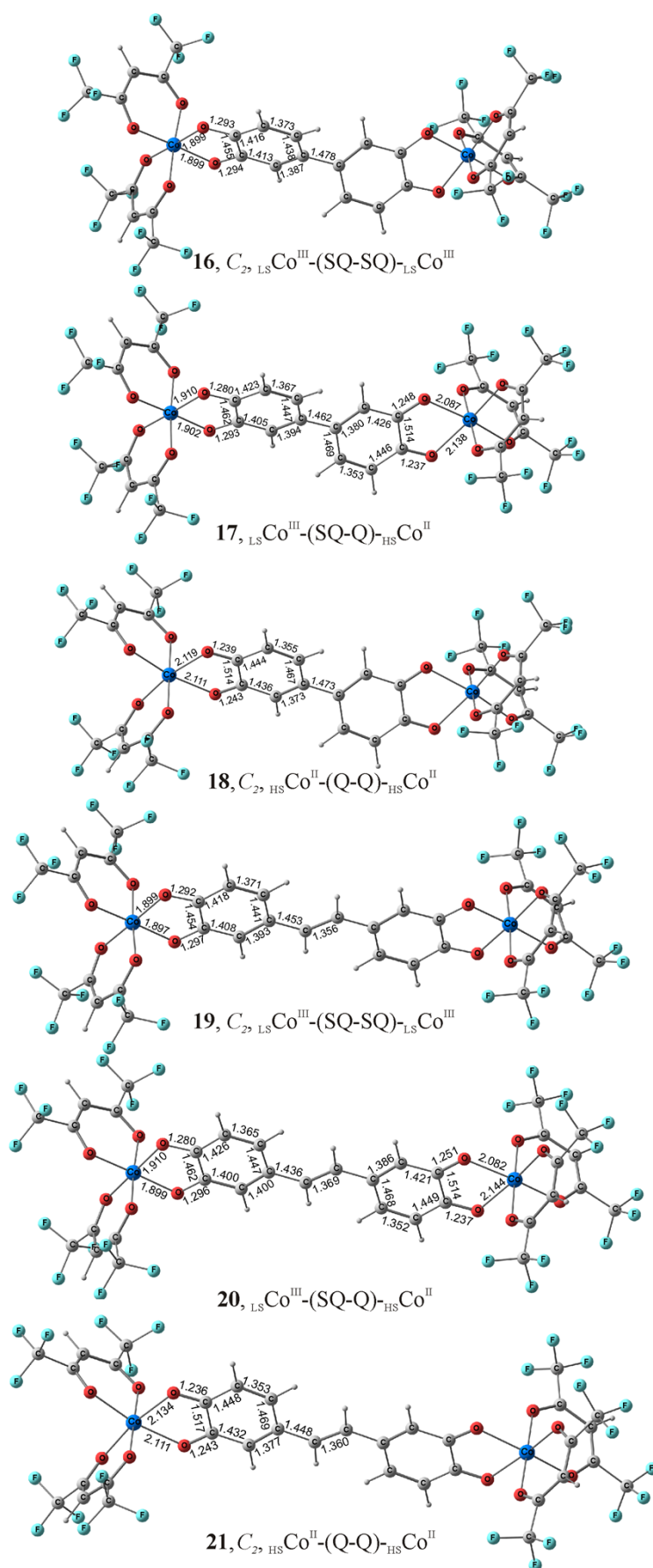


Fig. S4 Optimized geometries of the structures **16-21** of adduct **1** ($R = CF_3$; $R_1 = R_2 = H$; $X = \text{none}, HC=CH$) calculated by the B3LYP*/6-311++G(d,p) method.

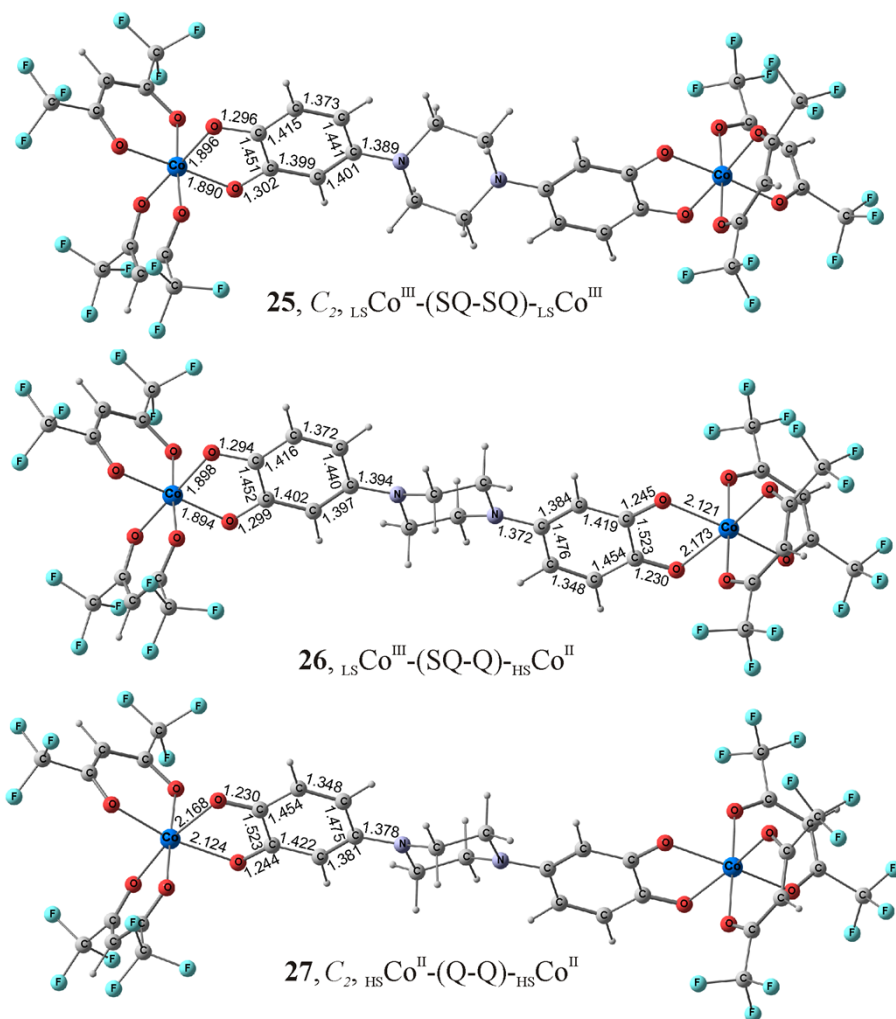


Fig. S5 Optimized geometries of the structures **25-27** of adduct **1** ($R = CF_3$; $R_1 = R_2 = H$; $X = \text{piperazindiyl}$) calculated by the B3LYP*/6-311++G(d,p) method.

Total energies and optimized geometries at B3LYP*/6-311++G(d,p)

Table S1. Total energies without (E) and with account (E_{ZPE}) taken for energies of zero harmonic vibrations (all energy values are given in a.u.) of the structures of Co(II) diketonates and di-*o*-quinones calculated by the DFT B3LYP*/6-311++G(d,p) method

Structure	E	E_{ZPE}
<i>bis</i> -(malonate)Co(II)	-1915.67070	-1915.55690
<i>bis</i> -(trifluoroacetylacetonate)Co(II)	-3263.63635	-3263.50515
L (X=none)	-761.44583	-761.29751
L (X= HC=CH)	-838.82298	-838.64139
L (X= H ₂ C-CH ₂)	-840.03813	-839.83360
L (X=piperazindiyl)	-1028.08960	-1027.81459
4,4'- <i>bis</i> -(3-methyl-6- <i>tert</i> -butyl-1,2-benzoquinone)	-1154.40699	-1153.98201

Table S2. Spin states (S) and total energies without (E) and with account (E_{ZPE}) taken for energies of zero harmonic vibrations (all energy values are given in a.u.) of the structures **4 – 15** calculated by the DFT B3LYP*/6-311++G(d,p) method.

Structure	S	E	E_{ZPE}
4	2/2	-4592.86226	-4592.47569
4 BS		-4592.86704	
5	4/2	-4592.84289	-4592.46082
5 BS		-4592.83979	
6	6/2	-4592.81460	-4592.43707
7	2/2	-4670.23695	-4669.81745
7 BS		-4670.24315	
8	4/2	-4670.21931	-4669.80436
8 BS		-4670.21560	
9	6/2	-4670.19124	-4669.78061
10	2/2	-4671.45080	-4671.00796
10 BS		-4671.45092	
11	4/2	-4671.42796	-4670.98970
11 BS		-4671.42789	
12	6/2	-4671.40401	-4670.97025
13	2/2	-4859.49488	-4858.98233
13 BS		-4859.49488	
14	4/2	-4859.47572	-4858.96745
14 BS		-4859.47572	
15	6/2	-4859.45522	-4858.95137

Table S3. Spin states (S) and total energies without (E) and with account (E_{ZPE}) taken for energies of zero harmonic vibrations (all energy values are given in a.u.) of the structures **16 – 27** calculated by the DFT B3LYP*/6-311++G(d,p) method.

Structure	S	E	E_{ZPE}
16	2/2	-7288.79252	-7288.37197
16 BS		-7288.79766	
17	4/2	-7288.78439	-7288.36779
17 BS		-7288.78241	
18	6/2	-7288.76617	-7288.35331
19	2/2	-7366.16828	-7365.71477
19 BS		-7366.17556	
20	4/2	-7366.16295	-7365.71328
20 BS		-7366.16113	
21	6/2	-7366.14627	-7365.70014
22	2/2	-7367.38282	-7366.90605
22 BS		-7367.38294	
23	4/2	-7367.37296	-7366.90004
23 BS		-7367.37292	
24	6/2	-7367.36082	-7366.89163
MECP₂₂₋₂₃		-7367.36611	
MECP₂₃₋₂₄		-7367.35524	
25	2/2	-7555.43187	-7554.88495
25 BS		-7555.43187	
26	4/2	-7555.42782	-7554.88452
26 BS		-7555.42782	
27	6/2	-7555.42129	-7554.88159

Table S4. Spin states (S) and total energies without (E) and with account (E_{ZPE}) taken for energies of zero harmonic vibrations (all energy values are given in a.u.) of the structures **28 – 33** calculated by the DFT B3LYP*/6-311++G(d,p) method.

Structure	S	E	E_{ZPE}
28	2/2	-4985.81661	-4985.15362
28 BS		-4985.81862	
29	4/2	-4985.79802	-4985.13932
29 BS		-4985.79710	
30	6/2	-4985.77479	-4985.12105
31	2/2	-7681.75100	-7681.05403
31 BS		-7681.75214	
32	4/2	-7681.74568	-7681.05252
32 BS		-7681.74528	
33	6/2	-7681.73498	-7681.04576

L (X=none)E= -761.44583 a.u., E_{ZPE}= -761.29751 a.u.

8	4.823565000	0.650234000	-0.062476000
8	3.709376000	-1.833970000	0.543781000
6	2.996440000	-0.893469000	0.256138000
6	1.531498000	-1.004769000	0.202300000
6	0.737442000	0.059273000	-0.093041000
6	1.345383000	1.367531000	-0.396458000
6	2.674533000	1.580086000	-0.395720000
6	3.620478000	0.498495000	-0.073083000
1	1.129947000	-1.981766000	0.451500000
1	0.678288000	2.181967000	-0.660377000
1	3.100899000	2.547939000	-0.642401000
8	-4.823564000	-0.650238000	-0.062469000
8	-3.709379000	1.833971000	0.543773000
6	-2.996440000	0.893461000	0.256163000
6	-1.531499000	1.004770000	0.202304000
6	-0.737441000	-0.059270000	-0.093041000
6	-1.345381000	-1.367531000	-0.396452000
6	-2.674531000	-1.580086000	-0.395720000
6	-3.620478000	-0.498489000	-0.073111000
1	-1.129949000	1.981767000	0.451503000
1	-0.678285000	-2.181967000	-0.660364000
1	-3.100896000	-2.547941000	-0.642397000

L (X= HC=CH)E= -838.82298 a.u., E_{ZPE}= -838.64139 a.u.

6	0.512886000	0.442776000	0.000436000
1	0.297913000	1.508172000	0.000350000
6	-0.512886000	-0.442779000	0.000448000
1	-0.297913000	-1.508175000	0.000378000
8	-5.940194000	0.852962000	0.000078000
8	-5.101187000	-1.807806000	-0.001690000
6	-4.284939000	-0.905700000	-0.000879000
6	-2.840372000	-1.142975000	-0.000444000
6	-1.931523000	-0.124136000	0.000348000
6	-2.398224000	1.274084000	0.001118000
6	-3.700842000	1.610101000	0.001010000
6	-4.758159000	0.581860000	0.000052000
1	-2.523639000	-2.182812000	-0.000935000
1	-1.653465000	2.063234000	0.001930000
1	-4.027362000	2.645955000	0.001694000
8	5.940195000	-0.852960000	0.000115000
8	5.101185000	1.807808000	-0.001680000
6	4.284938000	0.905701000	-0.000859000
6	2.840370000	1.142974000	-0.000450000
6	1.931524000	0.124134000	0.000333000
6	2.398226000	-1.274085000	0.001125000
6	3.700843000	-1.610101000	0.001012000
6	4.758160000	-0.581859000	-0.000042000
1	2.523637000	2.182810000	-0.000932000
1	1.653468000	-2.063236000	0.001956000

1	4.027365000	-2.645955000	0.001727000
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L (X= H₂C-CH₂)

E= -840.03813 a.u., E_{ZPE}= -839.83360 a.u.

8	5.887595000	0.731067000	-0.288660000
8	4.912818000	-1.871247000	-0.099002000
6	4.157981000	-0.927781000	0.026665000
6	2.718892000	-1.083960000	0.278349000
6	1.896701000	-0.016731000	0.405254000
6	2.429780000	1.351288000	0.306666000
6	3.729993000	1.623371000	0.084444000
6	4.708618000	0.533994000	-0.081196000
1	2.351802000	-2.104228000	0.356683000
1	1.724993000	2.170425000	0.434419000
1	4.108843000	2.639402000	0.023845000
8	-5.887661000	-0.730959000	0.288469000
8	-4.912812000	1.871311000	0.098549000
6	-4.157986000	0.927809000	-0.026921000
6	-2.718864000	1.083926000	-0.278470000
6	-1.896668000	0.016666000	-0.405087000
6	-2.429771000	-1.351330000	-0.306270000
6	-3.730009000	-1.623354000	-0.084127000
6	-4.708654000	-0.533936000	0.081133000
1	-2.351759000	2.104177000	-0.356960000
1	-1.724979000	-2.170500000	-0.433772000
1	-4.108871000	-2.639368000	-0.023335000
6	-0.414700000	0.173260000	-0.633711000
6	0.414742000	-0.173388000	0.633916000
1	-0.096605000	-0.488205000	-1.449949000
1	-0.199348000	1.198618000	-0.949894000
1	0.199435000	-1.198760000	0.950077000
1	0.096636000	0.488052000	1.450167000

L (X=piperazindiyl)

E= -1028.08960 a.u., E_{ZPE}= -1027.81459 a.u.

7	1.433940000	0.080729000	-0.048543000
6	0.640624000	1.036865000	0.735842000
6	-0.763158000	1.212601000	0.161364000
7	-1.433929000	-0.080894000	0.049053000
6	-0.640599000	-1.037035000	-0.735333000
6	0.763178000	-1.212774000	-0.160840000
1	1.133889000	2.008360000	0.763013000
1	0.562436000	0.678627000	1.775321000
1	-1.333854000	1.848517000	0.841619000
1	-0.711312000	1.716184000	-0.818291000
1	-1.133854000	-2.008531000	-0.762528000
1	-0.562390000	-0.678786000	-1.774805000
1	1.333888000	-1.848704000	-0.841069000
1	0.711305000	-1.716336000	0.818823000
8	-6.912362000	-0.597326000	0.089432000
8	-5.766700000	1.927373000	-0.182271000
6	-5.053033000	0.943586000	-0.071150000

6	-3.602048000	1.005088000	-0.084381000
6	-2.821913000	-0.117245000	-0.005086000
6	-3.452908000	-1.445061000	0.124726000
6	-4.785293000	-1.615774000	0.151798000
6	-5.706751000	-0.466078000	0.056134000
1	-3.180628000	1.996160000	-0.203453000
1	-2.807213000	-2.306927000	0.256509000
1	-5.234883000	-2.596471000	0.277234000
8	6.912238000	0.597225000	-0.093616000
8	5.766906000	-1.926933000	0.184671000
6	5.053132000	-0.943397000	0.071979000
6	3.602159000	-1.005086000	0.084894000
6	2.821923000	0.117174000	0.005449000
6	3.452772000	1.445044000	-0.124403000
6	4.785140000	1.615828000	-0.152098000
6	5.706685000	0.466100000	-0.057680000
1	3.180823000	-1.996137000	0.204441000
1	2.806970000	2.306905000	-0.255711000
1	5.234623000	2.596553000	-0.277691000

4,4'- bis-(3-methyl-6-tert-butyl-1,2-benzoquinone)

E= -1154.40699 a.u., E_{ZPE}= -1153.98201 a.u.

8	4.640268000	-1.332076000	-0.301613000
8	2.906745000	-2.746602000	-1.832164000
8	-4.640172000	1.332618000	-0.300422000
8	-2.907080000	2.746909000	-1.831640000
6	3.483168000	-0.965838000	-0.327931000
6	2.486984000	-1.776521000	-1.233890000
6	1.078089000	-1.338944000	-1.332497000
6	0.705816000	-0.251738000	-0.608994000
6	1.642196000	0.483507000	0.254308000
6	2.954521000	0.197279000	0.433969000
6	3.883876000	0.999270000	1.351325000
6	4.477948000	0.064087000	2.435258000
6	5.030520000	1.621335000	0.514649000
6	3.134017000	2.140514000	2.062656000
6	0.184089000	-2.135856000	-2.236592000
6	-3.483182000	0.966099000	-0.327311000
6	-2.487116000	1.776962000	-1.233310000
6	-1.078138000	1.339638000	-1.331881000
6	-0.705834000	0.252108000	-0.608880000
6	-1.642195000	-0.483555000	0.254082000
6	-2.954515000	-0.197438000	0.433925000
6	-3.883808000	-0.999922000	1.350923000
6	-4.477746000	-0.065379000	2.435493000
6	-5.030514000	-1.621449000	0.513958000
6	-3.133890000	-2.141591000	2.061502000
6	-0.184131000	2.137017000	-2.235553000
1	1.206084000	1.326271000	0.780767000
1	5.119943000	0.645008000	3.106735000
1	5.077931000	-0.733171000	1.993729000
1	3.683773000	-0.388559000	3.039767000

1	5.689105000	2.200890000	1.171410000
1	4.633717000	2.301570000	-0.247424000
1	5.628907000	0.854332000	0.020518000
1	3.833094000	2.680723000	2.708528000
1	2.322453000	1.766947000	2.697401000
1	2.716168000	2.865510000	1.355193000
1	0.147391000	-3.183157000	-1.916446000
1	-0.830951000	-1.736304000	-2.265787000
1	0.587390000	-2.146286000	-3.255485000
1	-1.206053000	-1.326549000	0.780146000
1	-5.119552000	-0.646741000	3.106770000
1	-3.683497000	0.386964000	3.040117000
1	-5.077863000	0.732077000	1.994507000
1	-5.689128000	-2.201355000	1.170390000
1	-5.628895000	-0.854148000	0.020273000
1	-4.633782000	-2.301283000	-0.248507000
1	-3.832960000	-2.682288000	2.706974000
1	-2.322381000	-1.768370000	2.696518000
1	-2.715944000	-2.866060000	1.353558000
1	0.830756000	1.737121000	-2.265401000
1	-0.587770000	2.148526000	-3.254296000
1	-0.146949000	3.184036000	-1.914498000

4 (R= H; R₁= R₂ = H; X=none)

E= -4592.86226 a.u., E_{ZPE}= -4592.47569 a.u.

27	5.710411000	0.010881000	0.088994000
8	5.851888000	-0.437783000	-1.760669000
8	6.713965000	-1.465575000	0.732717000
8	7.313115000	1.006232000	-0.114475000
8	5.403437000	0.489112000	1.910769000
6	6.477972000	-1.455519000	-2.179816000
6	7.150900000	-2.414266000	-1.417711000
6	7.216085000	-2.350185000	-0.025170000
6	7.818779000	1.708950000	0.812779000
6	7.339512000	1.875130000	2.112851000
6	6.173107000	1.252525000	2.565200000
1	7.637730000	-3.237770000	-1.926011000
1	7.890747000	2.510505000	2.795438000
8	4.626671000	1.505518000	-0.434238000
8	4.067063000	-0.977174000	0.157354000
6	3.070666000	-0.217815000	-0.149189000
6	1.726533000	-0.660603000	-0.170608000
6	0.705608000	0.220326000	-0.497403000
6	1.034844000	1.580180000	-0.826781000
6	2.327240000	2.046323000	-0.824492000
6	3.384601000	1.166665000	-0.480241000
1	0.233073000	2.252590000	-1.113018000
27	-5.710409000	-0.010862000	0.089029000
8	-5.403469000	-0.488878000	1.910866000
8	-7.313134000	-1.006199000	-0.114338000
8	-6.713936000	1.465696000	0.732560000
8	-5.851850000	0.437581000	-1.760690000

6	-6.173166000	-1.252191000	2.565382000
6	-7.339582000	-1.874822000	2.113094000
6	-7.818829000	-1.708787000	0.812996000
6	-7.216015000	2.350232000	-0.025439000
6	-7.150806000	2.414146000	-1.417987000
6	-6.477896000	1.455288000	-2.179968000
1	-7.890840000	-2.510100000	2.795752000
1	-7.637603000	3.237604000	-1.926393000
8	-4.067038000	0.977163000	0.157284000
8	-4.626700000	-1.505588000	-0.434010000
6	-3.384624000	-1.166764000	-0.480069000
6	-2.327285000	-2.046480000	-0.824240000
6	-1.034880000	-1.580360000	-0.826599000
6	-0.705613000	-0.220479000	-0.497359000
6	-1.726518000	0.660509000	-0.170667000
6	-3.070660000	0.217750000	-0.149186000
1	-0.233130000	-2.252814000	-1.112790000
1	-2.564733000	-3.071677000	-1.088840000
1	-1.529639000	1.688997000	0.111670000
1	1.529678000	-1.689059000	0.111862000
1	2.564664000	3.071498000	-1.089200000
1	-7.759246000	3.144507000	0.502885000
1	-6.474034000	1.575086000	-3.271434000
1	-8.740369000	-2.234708000	0.531542000
1	-5.863774000	-1.429909000	3.603771000
1	6.474127000	-1.575449000	-3.271268000
1	7.759329000	-3.144382000	0.503258000
1	8.740310000	2.234858000	0.531272000
1	5.863701000	1.430359000	3.603565000

5 (R= H; R₁= R₂ = H; X=none)

E= -4592.84289 a.u., E_{ZPE}= -4592.46082 a.u.

27	-5.821973000	-0.000826000	0.072367000
8	-4.488013000	-1.472646000	-0.695144000
8	-3.999257000	0.903257000	0.285466000
8	-6.054806000	0.615865000	-1.845684000
8	-6.854915000	1.619199000	0.670686000
8	-7.450406000	-1.177976000	-0.103793000
8	-5.617143000	-0.701430000	1.962329000
6	-2.998124000	0.228758000	-0.083433000
6	-1.654760000	0.673151000	-0.015273000
6	-0.609234000	-0.154290000	-0.403247000
6	-0.913392000	-1.490843000	-0.904336000
6	-2.179422000	-1.968938000	-1.014350000
6	-3.288945000	-1.139106000	-0.616153000
6	-6.826134000	1.531876000	-2.251630000
6	-7.576971000	2.411114000	-1.459675000
6	-7.526024000	2.404615000	-0.060787000
6	-8.026409000	-1.853913000	0.796624000
6	-7.601863000	-2.011555000	2.121978000
6	-6.422068000	-1.435009000	2.607179000
1	-1.483440000	1.658782000	0.401976000

1	-8.193654000	3.154609000	-1.952373000
1	-8.194850000	-2.626191000	2.789960000
1	-0.088896000	-2.110905000	-1.237701000
1	-2.391231000	-2.956021000	-1.412529000
1	-6.148370000	-1.644223000	3.653268000
1	-8.949069000	-2.372685000	0.492546000
1	-6.895279000	1.653448000	-3.344264000
1	-8.117221000	3.166326000	0.471298000
27	5.811343000	0.011747000	0.070902000
8	5.564384000	0.046706000	1.962177000
8	7.394890000	1.055746000	0.055747000
8	6.849654000	-1.550742000	0.315927000
8	5.889593000	0.018178000	-1.834487000
6	6.373399000	0.612215000	2.756358000
6	7.533958000	1.317660000	2.428038000
6	7.952064000	1.493741000	1.108625000
6	7.342836000	-2.216271000	-0.645821000
6	7.235556000	-1.947775000	-2.010524000
6	6.520039000	-0.853345000	-2.503096000
1	8.123490000	1.753382000	3.225498000
1	7.720947000	-2.613803000	-2.713461000
8	4.182368000	-0.994407000	-0.048867000
8	4.680344000	1.568161000	-0.055030000
6	3.453574000	1.226593000	-0.147291000
6	2.375883000	2.154226000	-0.250578000
6	1.094820000	1.685003000	-0.326866000
6	0.783671000	0.272915000	-0.323049000
6	1.832070000	-0.646892000	-0.241378000
6	3.162974000	-0.208280000	-0.146262000
1	0.282852000	2.395547000	-0.431407000
1	2.602021000	3.215054000	-0.275913000
1	1.657236000	-1.715606000	-0.199420000
1	7.914731000	-3.100143000	-0.335918000
1	6.480774000	-0.709902000	-3.590751000
1	8.864119000	2.077169000	0.928750000
1	6.104299000	0.527092000	3.817243000

6 (R= H; R₁= R₂ = H; X=none)

E= -4592.81460 a.u., E_{ZPE}= -4592.43707 a.u.

27	-5.929635000	-0.023289000	0.078432000
8	-4.587462000	-1.558784000	-0.418013000
8	-4.067363000	0.933072000	0.203841000
8	-6.076024000	0.338839000	-1.903500000
8	-6.990125000	1.654431000	0.404355000
8	-7.537335000	-1.231255000	0.050874000
8	-5.764786000	-0.384022000	2.058356000
6	-3.084753000	0.207734000	-0.080061000
6	-1.727546000	0.657829000	-0.099807000
6	-0.702854000	-0.219332000	-0.384439000
6	-1.013613000	-1.611037000	-0.683268000
6	-2.282881000	-2.099765000	-0.701408000
6	-3.384207000	-1.222839000	-0.409734000

6	-6.805674000	1.204945000	-2.470040000
6	-7.578419000	2.188762000	-1.841896000
6	-7.604401000	2.355320000	-0.451571000
6	-8.159188000	-1.706551000	1.045365000
6	-7.786075000	-1.603055000	2.391157000
6	-6.609180000	-0.965153000	2.801487000
1	-1.549103000	1.695109000	0.160987000
1	-8.153104000	2.870963000	-2.458222000
1	-8.415298000	-2.066933000	3.142408000
1	-0.192349000	-2.273203000	-0.935518000
1	-2.497565000	-3.134004000	-0.949922000
1	-6.374471000	-0.976604000	3.877043000
1	-9.078800000	-2.265589000	0.813457000
1	-6.812730000	1.180483000	-3.570707000
1	-8.208104000	3.183431000	-0.049272000
27	5.929651000	0.023337000	0.078407000
8	4.587465000	1.558320000	-0.419710000
8	4.067393000	-0.932872000	0.204862000
8	6.076091000	-0.340879000	-1.903131000
8	6.990102000	-1.654017000	0.406155000
8	7.537363000	1.231264000	0.049564000
8	5.764743000	0.386212000	2.057927000
6	3.084771000	-0.207848000	-0.079840000
6	1.727576000	-0.657995000	-0.099169000
6	0.702867000	0.218875000	-0.384650000
6	1.013608000	1.610275000	-0.684880000
6	2.282873000	2.099001000	-0.703515000
6	3.384209000	1.222378000	-0.410985000
6	6.805751000	-1.207603000	-2.468717000
6	7.578519000	-2.190714000	-1.839494000
6	7.604409000	-2.355829000	-0.449001000
6	8.159090000	1.707789000	1.043547000
6	7.785919000	1.605786000	2.389434000
6	6.609032000	0.968303000	2.800429000
1	1.549136000	-1.695021000	0.162639000
1	8.153309000	-2.873507000	-2.455067000
1	8.415102000	2.070513000	3.140192000
1	0.192359000	2.272205000	-0.937782000
1	2.497540000	3.132995000	-0.953057000
1	6.374304000	0.980905000	3.875965000
1	9.078742000	2.266519000	0.811061000
1	6.812946000	-1.184241000	-3.569405000
1	8.208168000	-3.183446000	-0.045780000

7 (R= H; R₁= R₂ = H; X= HC=CH)

E= -4670.23695 a.u., E_{ZPE}= -4669.81745 a.u.

27	-6.974477000	0.010870000	-0.014065000
8	-6.924277000	-1.896816000	-0.017706000
8	-8.053367000	0.189648000	-1.565006000
8	-8.537980000	-0.118590000	1.055888000
8	-6.860466000	1.915841000	0.022917000
6	-7.515886000	-2.602146000	-0.886947000

6	-8.276247000	-2.155790000	-1.971227000
6	-8.484251000	-0.800515000	-2.230595000
6	-9.144611000	0.890427000	1.527909000
6	-8.812597000	2.235970000	1.364225000
6	-7.699293000	2.647518000	0.626590000
1	-8.717813000	-2.888404000	-2.635936000
1	-9.436754000	2.988400000	1.830930000
8	-5.825339000	-0.038504000	1.523148000
8	-5.360018000	0.008450000	-1.047551000
6	-4.326979000	-0.017474000	-0.272954000
6	-2.993769000	-0.021879000	-0.735296000
6	-1.931602000	-0.049968000	0.164670000
6	-2.213855000	-0.080016000	1.576515000
6	-3.495281000	-0.078364000	2.064739000
6	-4.590816000	-0.046123000	1.160466000
1	-1.388587000	-0.106813000	2.279846000
27	6.974435000	0.010935000	0.013985000
8	6.860442000	1.915854000	-0.025673000
8	8.537790000	-0.120055000	-1.056015000
8	8.053437000	0.191955000	1.564614000
8	6.924271000	-1.896742000	0.020363000
6	7.699287000	2.646676000	-0.630352000
6	8.812529000	2.234078000	-1.367496000
6	9.144435000	0.888300000	-1.529434000
6	8.484609000	-0.797259000	2.231423000
6	8.276777000	-2.152910000	1.973883000
6	7.516190000	-2.600823000	0.890407000
1	9.436697000	2.985846000	-1.835252000
1	8.718594000	-2.884568000	2.639478000
8	5.360068000	0.009969000	1.047628000
8	5.825176000	-0.040676000	-1.523039000
6	4.590683000	-0.047875000	-1.160239000
6	3.495084000	-0.081526000	-2.064373000
6	2.213701000	-0.082572000	-1.576038000
6	1.931553000	-0.050473000	-0.164218000
6	2.993786000	-0.021054000	0.735623000
6	4.326962000	-0.017184000	0.273160000
1	1.388380000	-0.110539000	-2.279259000
1	3.700797000	-0.107792000	-3.129547000
1	2.820253000	0.003840000	1.807290000
1	-2.820153000	0.001494000	-1.806985000
1	-3.701076000	-0.103048000	3.129935000
1	9.088369000	-0.524962000	3.106902000
1	7.400133000	-3.684409000	0.755973000
1	10.028477000	0.643781000	-2.132665000
1	7.503968000	3.724449000	-0.553066000
1	-7.399762000	-3.685536000	-0.750997000
1	-9.087919000	-0.529468000	-3.106525000
1	-10.028750000	0.646765000	2.131344000
1	-7.503910000	3.725176000	0.547868000
6	0.574963000	-0.049095000	0.359192000
1	0.515489000	-0.043899000	1.445437000

6	-0.574991000	-0.049340000	-0.358671000
1	-0.515495000	-0.045245000	-1.444920000

8 (R= H; R₁= R₂ = H; X= HC=CH)

E= -4670.21931 a.u., E_{ZPE}= -4669.80436 a.u.

27	7.050113000	0.002357000	0.004071000
8	6.949740000	1.908164000	0.027358000
8	8.604502000	-0.102665000	-1.081158000
8	8.139533000	0.120854000	1.545806000
8	6.982583000	-1.902421000	-0.060107000
6	7.804154000	2.653812000	-0.537279000
6	8.918748000	2.258634000	-1.281487000
6	9.230235000	0.916812000	-1.504498000
6	8.566394000	-0.895331000	2.175126000
6	8.345654000	-2.239184000	1.872766000
6	7.574446000	-2.642843000	0.779715000
1	9.557255000	3.021388000	-1.710373000
1	8.786142000	-2.996787000	2.509441000
8	5.445129000	-0.022229000	1.050035000
8	5.873656000	0.011280000	-1.524525000
6	4.653288000	-0.003338000	-1.152724000
6	3.551493000	-0.002854000	-2.061883000
6	2.277534000	-0.012792000	-1.571777000
6	2.003571000	-0.023972000	-0.151713000
6	3.076962000	-0.027491000	0.750308000
6	4.399426000	-0.018110000	0.290210000
1	1.448659000	-0.011493000	-2.270851000
1	3.759686000	0.005285000	-3.126744000
1	2.900312000	-0.034874000	1.821627000
1	9.178056000	-0.656976000	3.054598000
1	7.448455000	-3.719648000	0.607006000
1	10.112068000	0.685828000	-2.115941000
1	7.620323000	3.729458000	-0.416551000
6	0.665307000	-0.030919000	0.361204000
1	0.599540000	-0.036815000	1.446647000
6	-0.497821000	-0.030300000	-0.365838000
1	-0.433199000	-0.024419000	-1.451249000
27	-7.067150000	0.006584000	-0.040016000
8	-5.677102000	-0.075324000	1.575550000
8	-5.269000000	0.001634000	-1.008055000
8	-7.154197000	-2.017274000	0.086762000
8	-8.153313000	-0.097796000	-1.731843000
8	-8.675239000	0.156704000	1.171847000
8	-7.007590000	2.033565000	-0.079738000
6	-4.239924000	-0.023676000	-0.274572000
6	-2.906844000	-0.030247000	-0.740580000
6	-1.834084000	-0.035618000	0.149947000
6	-2.096994000	-0.043221000	1.585034000
6	-3.353911000	-0.046132000	2.095380000
6	-4.488539000	-0.048236000	1.201787000
6	-7.891548000	-2.781642000	-0.599083000
6	-8.703531000	-2.417899000	-1.681947000

6	-8.764648000	-1.111235000	-2.180417000
6	-9.320219000	1.197859000	1.486303000
6	-9.001117000	2.515706000	1.135090000
6	-7.861834000	2.840831000	0.389214000
1	-2.738796000	-0.019984000	-1.813437000
1	-9.279463000	-3.189895000	-2.180191000
1	-9.645262000	3.317312000	1.478914000
1	-1.255193000	-0.047853000	2.268820000
1	-3.544501000	-0.055260000	3.163798000
1	-7.671601000	3.908228000	0.194667000
1	-10.216418000	1.039860000	2.106859000
1	-7.874615000	-3.846627000	-0.317620000
1	-9.398243000	-0.935739000	-3.064068000

9 (R= H; R₁= R₂ = H; X= HC=CH)

E= -4670.19124 a.u., E_{ZPE}= -4669.78061 a.u.

6	-0.574265000	0.010005000	-0.363618000
1	-0.511211000	0.006215000	-1.448994000
6	0.574266000	0.010167000	0.364022000
1	0.511211000	0.006565000	1.449403000
27	7.179661000	-0.005227000	0.012366000
8	5.778150000	0.004158000	-1.569224000
8	5.343285000	0.003122000	1.016899000
8	7.186498000	-2.019578000	-0.168932000
8	8.278815000	-0.204367000	1.686523000
8	8.772036000	0.179640000	-1.206952000
8	7.146560000	2.012308000	0.171823000
6	4.331136000	0.002955000	0.276532000
6	2.982561000	-0.007668000	0.740180000
6	1.926753000	0.011683000	-0.152148000
6	2.196964000	0.038396000	-1.585862000
6	3.455355000	0.045331000	-2.095530000
6	4.587059000	0.018623000	-1.202463000
6	7.896775000	-2.837521000	0.486281000
6	8.730921000	-2.541782000	1.571185000
6	8.850093000	-1.252722000	2.105683000
6	9.451087000	1.222536000	-1.434718000
6	9.168839000	2.518568000	-0.984936000
6	8.031014000	2.824664000	-0.228658000
1	2.814341000	-0.023418000	1.812926000
1	9.278230000	-3.351284000	2.041141000
1	9.840411000	3.323099000	-1.263083000
1	1.357052000	0.055108000	-2.271954000
1	3.645251000	0.064000000	-3.163837000
1	7.869969000	3.880682000	0.038860000
1	10.346484000	1.085368000	-2.060774000
1	7.831359000	-3.890481000	0.170703000
1	9.494982000	-1.127041000	2.989321000
27	-7.179677000	-0.005234000	-0.012461000
8	-5.778254000	0.004034000	1.569307000
8	-5.343219000	0.003037000	-1.016789000
8	-7.186653000	-2.019587000	0.168793000

8	-8.278698000	-0.204255000	-1.686730000
8	-8.772101000	0.179712000	1.206817000
8	-7.146411000	2.012308000	-0.171846000
6	-4.331127000	0.002805000	-0.276362000
6	-2.982489000	-0.007827000	-0.739902000
6	-1.926766000	0.011486000	0.152533000
6	-2.197061000	0.038080000	1.586221000
6	-3.455500000	0.045032000	2.095773000
6	-4.587158000	0.018433000	1.202620000
6	-7.896904000	-2.837473000	-0.486519000
6	-8.730915000	-2.541659000	-1.571506000
6	-8.849973000	-1.252576000	-2.105978000
6	-9.451075000	1.222658000	1.434573000
6	-9.168714000	2.518680000	0.984823000
6	-8.030832000	2.824715000	0.228610000
1	-2.814200000	-0.023528000	-1.812631000
1	-9.278213000	-3.351120000	-2.041546000
1	-9.840243000	3.323251000	1.262958000
1	-1.357231000	0.054652000	2.272403000
1	-3.645512000	0.063607000	3.164065000
1	-7.869702000	3.880729000	-0.038874000
1	-10.346508000	1.085557000	2.060594000
1	-7.831581000	-3.890447000	-0.170966000
1	-9.494766000	-1.126846000	-2.989680000

10 (R= H; R₁= R₂ = H; X= H₂C-CH₂)

E= -4671.45080 a.u., E_{ZPE}= -4671.00796 a.u.

27	6.818297000	0.026068000	-0.012089000
8	6.513835000	1.765437000	0.713362000
8	7.839265000	0.605669000	-1.504194000
8	8.400313000	-0.043065000	1.036134000
8	6.959790000	-1.745666000	-0.707563000
6	6.962210000	2.824286000	0.183483000
6	7.722211000	2.936107000	-0.983831000
6	8.099173000	1.824577000	-1.739027000
6	9.149610000	-1.064337000	1.101078000
6	8.985967000	-2.282855000	0.440564000
6	7.908143000	-2.531409000	-0.413625000
1	8.028143000	3.920932000	-1.315606000
1	9.719332000	-3.064629000	0.597316000
8	5.746463000	-0.670846000	1.417872000
8	5.171355000	0.192718000	-0.978933000
6	4.180226000	-0.211698000	-0.259003000
6	2.833324000	-0.212724000	-0.698147000
6	1.831484000	-0.658168000	0.141388000
6	2.162925000	-1.123071000	1.456883000
6	3.455648000	-1.144760000	1.923988000
6	4.502094000	-0.688923000	1.080874000
1	1.359035000	-1.477439000	2.097408000
27	-6.818293000	-0.019074000	0.015625000
8	-6.520845000	-1.794379000	-0.619364000
8	-8.427921000	0.273357000	-0.949934000

8	-7.815191000	-0.784318000	1.438845000
8	-6.954250000	1.786015000	0.620521000
6	-7.300739000	-2.380088000	-1.426907000
6	-8.471403000	-1.874367000	-1.998529000
6	-8.943889000	-0.590595000	-1.721760000
6	-8.313916000	-0.102840000	2.385212000
6	-8.247806000	1.279489000	2.565118000
6	-7.576538000	2.118694000	1.671686000
1	-9.031087000	-2.500787000	-2.682569000
1	-8.731548000	1.717426000	3.429851000
8	-5.172412000	-0.172961000	0.986078000
8	-5.741872000	0.629019000	-1.433450000
6	-4.498015000	0.653345000	-1.094867000
6	-3.449491000	1.087240000	-1.946955000
6	-2.156721000	1.067411000	-1.480015000
6	-1.826851000	0.623677000	-0.156764000
6	-2.830854000	0.201672000	0.692137000
6	-4.178372000	0.202547000	0.254616000
1	-1.351471000	1.406059000	-2.127283000
6	0.385310000	-0.632603000	-0.289314000
6	-0.380406000	0.597080000	0.272904000
1	0.325274000	-0.625299000	-1.382829000
1	-0.121869000	-1.543783000	0.050617000
1	0.126934000	1.508110000	-0.067577000
1	-0.319520000	0.590142000	1.366362000
1	-3.695854000	1.430780000	-2.946365000
1	-2.617880000	-0.134379000	1.702883000
1	2.619361000	0.138369000	-1.703589000
1	3.703133000	-1.503214000	2.917865000
1	-8.854612000	-0.695372000	3.134734000
1	-7.570776000	3.196207000	1.883191000
1	-9.868558000	-0.263787000	-2.215168000
1	-6.997396000	-3.401083000	-1.694089000
1	6.708217000	3.746783000	0.722311000
1	8.691541000	1.994988000	-2.647507000
1	10.019887000	-0.947373000	1.760004000
1	7.851436000	-3.515484000	-0.897537000

11 (R= H; R₁= R₂ = H; X= H₂C–CH₂)

E= -4671.42796 a.u., E_{ZPE}= -4670.98970 a.u.

27	6.906494000	0.022304000	-0.016711000
8	5.682648000	-0.642358000	1.489214000
8	5.112057000	0.110497000	-0.961996000
8	6.638900000	1.766871000	0.669237000
8	7.903568000	0.667677000	-1.618253000
8	8.539574000	-0.113522000	1.094262000
8	7.063798000	-1.743776000	-0.681619000
6	4.129539000	-0.245898000	-0.224288000
6	2.775758000	-0.253990000	-0.651117000
6	1.770998000	-0.665242000	0.201877000
6	2.099900000	-1.088941000	1.530328000
6	3.392762000	-1.099735000	1.996480000

6	4.452474000	-0.676376000	1.147199000
6	7.138332000	2.825720000	0.175849000
6	7.911679000	2.961106000	-0.977038000
6	8.225631000	1.875562000	-1.804629000
6	9.321694000	-1.107947000	1.081383000
6	9.161149000	-2.287192000	0.345415000
6	8.045335000	-2.518224000	-0.460355000
1	2.560565000	0.064077000	-1.667450000
1	8.248474000	3.951339000	-1.259888000
1	9.907697000	-3.067496000	0.432764000
1	1.295069000	-1.419266000	2.182776000
1	3.636278000	-1.426413000	3.002464000
6	0.325062000	-0.645252000	-0.231091000
6	-0.438067000	0.600266000	0.298732000
1	0.266339000	-0.664971000	-1.324644000
1	-0.186182000	-1.545947000	0.130442000
1	0.075476000	1.500923000	-0.059471000
1	-0.383150000	0.617568000	1.392389000
1	7.970100000	-3.487995000	-0.968886000
1	10.207163000	-1.024756000	1.727805000
1	6.901431000	3.734229000	0.744516000
1	8.802857000	2.081018000	-2.718086000
27	-6.874306000	-0.015821000	0.004362000
8	-6.569828000	-1.798746000	-0.605843000
8	-8.476966000	0.262274000	-0.977651000
8	-7.881839000	-0.764508000	1.429323000
8	-7.017088000	1.796645000	0.585551000
6	-7.340951000	-2.394533000	-1.414327000
6	-8.506630000	-1.896882000	-2.003053000
6	-8.984015000	-0.611013000	-1.744785000
6	-8.386578000	-0.072076000	2.364383000
6	-8.321792000	1.312332000	2.528402000
6	-7.645760000	2.141288000	1.628980000
1	-9.058725000	-2.531732000	-2.685506000
1	-8.810877000	1.760259000	3.384990000
8	-5.236246000	-0.155995000	0.989199000
8	-5.787977000	0.615098000	-1.444240000
6	-4.546276000	0.643291000	-1.097151000
6	-3.491735000	1.065772000	-1.947333000
6	-2.202271000	1.050913000	-1.471120000
6	-1.881718000	0.623994000	-0.139965000
6	-2.892171000	0.213533000	0.707125000
6	-4.236412000	0.209637000	0.260147000
1	-1.391976000	1.380066000	-2.116945000
1	-3.730886000	1.396539000	-2.952799000
1	-2.686223000	-0.110190000	1.723326000
1	-8.932111000	-0.655732000	3.117403000
1	-7.642200000	3.221281000	1.827613000
1	-9.904804000	-0.291621000	-2.250240000
1	-7.033834000	-3.418138000	-1.666901000

12 (R= H; R₁= R₂ = H; X= H₂C–CH₂)

E= -4671.40401 a.u., E_{ZPE}= -4670.97025 a.u.

27	7.036120000	0.000740000	-0.011862000
8	5.702849000	-0.337641000	1.575471000
8	5.174256000	-0.043472000	-0.970901000
8	6.881126000	1.975477000	0.403699000
8	8.056638000	0.486033000	-1.679972000
8	8.681032000	-0.176150000	1.136533000
8	7.178889000	-1.976848000	-0.421779000
6	4.194363000	-0.234095000	-0.216777000
6	2.827227000	-0.281643000	-0.650026000
6	1.828074000	-0.524485000	0.252147000
6	2.144393000	-0.736881000	1.655508000
6	3.414807000	-0.697686000	2.142900000
6	4.502578000	-0.427057000	1.240756000
6	7.504340000	2.919689000	-0.164425000
6	8.325369000	2.822889000	-1.294426000
6	8.528784000	1.620100000	-1.982865000
6	9.464058000	-1.167619000	1.206647000
6	9.288182000	-2.417527000	0.599659000
6	8.153518000	-2.739394000	-0.155032000
1	2.624256000	-0.133610000	-1.706703000
1	8.791579000	3.724481000	-1.675945000
1	10.043544000	-3.180186000	0.752918000
1	1.319910000	-0.944107000	2.333560000
1	3.640667000	-0.860555000	3.191713000
1	8.082793000	-3.765129000	-0.549568000
1	10.366550000	-1.023986000	1.821041000
1	7.365509000	3.919845000	0.275241000
1	9.151798000	1.654054000	-2.890310000
27	-7.032804000	-0.029656000	-0.009596000
8	-5.704544000	0.578940000	-1.515396000
8	-5.177762000	-0.073138000	0.963328000
8	-7.312904000	1.932251000	0.397551000
8	-8.085902000	-0.468991000	1.650417000
8	-8.635115000	-0.063777000	-1.230448000
8	-6.746598000	-1.990436000	-0.424662000
6	-4.201450000	0.261845000	0.256012000
6	-2.843527000	0.325059000	0.714917000
6	-1.841518000	0.673070000	-0.149105000
6	-2.147124000	0.994987000	-1.533381000
6	-3.411406000	0.971981000	-2.037946000
6	-4.503529000	0.614136000	-1.172609000
6	-8.106147000	2.422705000	1.253525000
6	-8.856036000	1.717902000	2.203041000
6	-8.779378000	0.326986000	2.347987000
6	-9.196586000	-1.081930000	-1.729216000
6	-8.747401000	-2.406456000	-1.653729000
6	-7.549245000	-2.764488000	-1.024171000
1	-2.647411000	0.082678000	1.755422000
1	-9.492049000	2.276262000	2.880860000
1	-9.332192000	-3.181499000	-2.136443000
1	-1.319911000	1.277666000	-2.180169000

1	-3.630584000	1.227145000	-3.069640000
1	-7.255706000	-3.825275000	-1.061836000
1	-10.126329000	-0.892165000	-2.287974000
1	-8.194838000	3.520362000	1.252538000
1	-9.368907000	-0.132350000	3.156778000
6	-0.399409000	0.704636000	0.289747000
6	0.380543000	-0.560435000	-0.167669000
1	0.096009000	1.590153000	-0.127047000
1	-0.348226000	0.792608000	1.379602000
1	0.315823000	-0.657389000	-1.256034000
1	-0.108419000	-1.443981000	0.261815000

13 (R= H; R₁= R₂= H; X= piperazindiyl)

E= -4859.49488 a.u., E_{ZPE}= -4858.98233 a.u.

7	1.394353000	-0.323472000	0.025290000
6	0.457033000	-1.387419000	-0.345045000
6	-0.963162000	-1.078502000	0.125169000
7	-1.399123000	0.221286000	-0.375277000
6	-0.458506000	1.286712000	-0.013156000
6	0.962274000	0.975228000	-0.479816000
1	0.772428000	-2.335357000	0.089356000
1	0.454977000	-1.510406000	-1.441419000
1	-1.626940000	-1.851394000	-0.268378000
1	-1.006569000	-1.114737000	1.227552000
1	-0.773835000	2.231317000	-0.455492000
1	-0.455947000	1.418763000	1.082311000
1	1.623404000	1.749543000	-0.085760000
1	1.010522000	1.007939000	-1.581881000
27	7.752914000	0.051540000	0.022808000
8	7.771982000	-0.850666000	-1.660710000
8	9.405400000	-0.658596000	0.647994000
8	8.693245000	1.470842000	-0.822257000
8	7.578684000	0.906694000	1.721703000
6	8.711658000	-1.616902000	-2.024292000
6	9.861783000	-1.956587000	-1.306157000
6	10.119921000	-1.458256000	-0.027935000
6	8.979889000	2.559405000	-0.239117000
6	8.698975000	2.918088000	1.080420000
6	8.024678000	2.066783000	1.960451000
1	10.576429000	-2.635187000	-1.756224000
1	9.015703000	3.891376000	1.435628000
8	6.057786000	0.791301000	-0.465093000
8	6.754817000	-1.417383000	0.746505000
6	5.489564000	-1.214859000	0.590968000
6	4.481946000	-2.110241000	1.029706000
6	3.158869000	-1.807903000	0.819665000
6	2.755988000	-0.598685000	0.150787000
6	3.734937000	0.294488000	-0.291720000
6	5.095971000	0.015889000	-0.078973000
1	2.401958000	-2.476932000	1.211946000
1	4.778697000	-3.015491000	1.549411000
1	3.491687000	1.201648000	-0.830073000

1	9.512277000	3.285391000	-0.867847000
1	7.847386000	2.422608000	2.984342000
1	11.042063000	-1.780575000	0.473755000
1	8.582605000	-2.054859000	-3.023296000
27	-7.751036000	-0.029306000	0.064969000
8	-7.780056000	-0.966363000	-1.599491000
8	-9.413261000	0.864995000	-0.182002000
8	-8.668361000	-1.513277000	0.819889000
8	-7.565861000	0.946388000	1.696509000
6	-8.726513000	-0.865667000	-2.434033000
6	-9.879977000	-0.083902000	-2.325293000
6	-10.134696000	0.722479000	-1.214573000
6	-8.939050000	-1.608283000	2.054762000
6	-8.654578000	-0.684932000	3.062359000
6	-7.994623000	0.520667000	2.808607000
1	-10.600465000	-0.101424000	-3.134199000
1	-8.957632000	-0.910489000	4.077753000
8	-6.042471000	-0.821324000	0.403737000
8	-6.778652000	1.382285000	-0.793935000
6	-5.509744000	1.158776000	-0.718109000
6	-4.517931000	2.030127000	-1.234711000
6	-3.189507000	1.709867000	-1.099967000
6	-2.765326000	0.504645000	-0.437605000
6	-3.727272000	-0.371124000	0.069620000
6	-5.095039000	-0.071180000	-0.059305000
1	-2.446024000	2.361094000	-1.544727000
1	-4.832616000	2.934218000	-1.745787000
1	-3.464005000	-1.276677000	0.601285000
1	-9.459505000	-2.533349000	2.336090000
1	-7.813708000	1.195147000	3.656354000
1	-11.060450000	1.313121000	-1.208372000
1	-8.601128000	-1.471741000	-3.341413000

14 (R= H; R₁= R₂ = H; X= piperazindiyl)

E= -4859.47572 a.u., E_{ZPE}= -4858.96745 a.u.

7	-1.483396000	0.114399000	0.336408000
6	-0.546858000	1.217349000	0.565555000
6	0.869627000	0.709709000	0.827987000
7	1.314836000	-0.164057000	-0.257845000
6	0.363189000	-1.254881000	-0.513678000
6	-1.049277000	-0.732421000	-0.767687000
1	-0.866372000	1.812963000	1.420189000
1	-0.534359000	1.883649000	-0.314112000
1	1.537020000	1.571786000	0.884100000
1	0.907723000	0.178147000	1.792722000
1	0.682336000	-1.845017000	-1.372018000
1	0.346511000	-1.925571000	0.360321000
1	-1.716729000	-1.593496000	-0.842285000
1	-1.082010000	-0.188143000	-1.727687000
27	-7.846373000	-0.009822000	-0.038219000
8	-7.777581000	1.642143000	-0.993487000
8	-9.508637000	0.325882000	0.822482000

8	-8.772924000	-0.737554000	-1.528215000
8	-7.755985000	-1.636215000	0.958533000
6	-8.687676000	2.519678000	-0.924412000
6	-9.860065000	2.473920000	-0.165255000
6	-10.179713000	1.388110000	0.651562000
6	-9.117961000	-1.955298000	-1.606085000
6	-8.909055000	-2.961586000	-0.661544000
6	-8.247102000	-2.727876000	0.546882000
1	-10.543059000	3.313740000	-0.208561000
1	-9.271217000	-3.960284000	-0.873919000
8	-6.139107000	-0.438067000	-0.795285000
8	-6.857336000	0.818451000	1.381938000
6	-5.590682000	0.685994000	1.179184000
6	-4.590490000	1.176070000	2.056853000
6	-3.264490000	0.989676000	1.753377000
6	-2.851727000	0.314866000	0.551832000
6	-3.818831000	-0.176672000	-0.324445000
6	-5.186172000	-0.014206000	-0.031733000
1	-2.513912000	1.319247000	2.462547000
1	-4.896887000	1.673095000	2.971486000
1	-3.564845000	-0.665107000	-1.256678000
1	-9.640263000	-2.220545000	-2.534702000
1	-8.123122000	-3.573315000	1.236794000
1	-11.115075000	1.432090000	1.224874000
1	-8.508993000	3.411457000	-1.539974000
27	7.900629000	0.029271000	0.023522000
8	6.622257000	-0.858243000	-1.433762000
8	5.961295000	0.491065000	0.723559000
8	7.891762000	-1.778972000	0.957309000
8	8.873026000	0.809176000	1.619565000
8	9.594129000	-0.416180000	-0.995131000
8	7.863937000	1.835955000	-0.923980000
6	5.018744000	0.053311000	0.027753000
6	3.639657000	0.201661000	0.339942000
6	2.667938000	-0.332122000	-0.488232000
6	3.063709000	-1.040405000	-1.709390000
6	4.358481000	-1.224033000	-2.060239000
6	5.410911000	-0.712415000	-1.210646000
6	8.554640000	-2.084057000	1.991112000
6	9.310900000	-1.221467000	2.794622000
6	9.400269000	0.159044000	2.566494000
6	10.310397000	0.391255000	-1.653802000
6	10.014685000	1.727771000	-1.954188000
6	8.811912000	2.346325000	-1.587444000
1	3.400345000	0.714489000	1.262596000
1	9.819206000	-1.635103000	3.658995000
1	10.731198000	2.296724000	-2.536810000
1	2.286683000	-1.387590000	-2.380406000
1	4.639001000	-1.734154000	-2.976099000
1	8.659984000	3.384497000	-1.926192000
1	11.260057000	-0.012528000	-2.041411000
1	8.513463000	-3.142932000	2.295015000

1	9.979878000	0.751049000	3.293673000
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15 (R= H; R₁= R₂= H; X= piperazindiyl)

E= -4859.45522 a.u., E_{ZPE}= -4858.95137 a.u.

7	-1.402892000	0.096743000	0.311938000
6	-0.450386000	1.060810000	0.876516000
6	0.956997000	0.476329000	0.981370000
7	1.399601000	-0.028819000	-0.316463000
6	0.446835000	-0.993216000	-0.880161000
6	-0.960027000	-0.408368000	-0.985774000
1	-0.772541000	1.378836000	1.867358000
1	-0.421507000	1.957887000	0.236931000
1	1.630535000	1.273287000	1.302249000
1	0.980070000	-0.322057000	1.741344000
1	0.768960000	-1.312621000	-1.870527000
1	0.417537000	-1.889593000	-0.239535000
1	-1.633804000	-1.205036000	-1.306810000
1	-0.982647000	0.389988000	-1.745724000
27	7.981980000	0.004479000	0.028496000
8	6.712825000	-0.380636000	-1.628584000
8	6.047719000	0.249705000	0.832501000
8	7.953014000	-2.001502000	0.357231000
8	8.939128000	0.238598000	1.793199000
8	9.680961000	-0.127952000	-1.060383000
8	7.975446000	2.009820000	-0.321713000
6	5.106097000	0.051999000	0.032246000
6	3.725878000	0.109261000	0.372230000
6	2.756592000	-0.135302000	-0.582990000
6	3.152208000	-0.440900000	-1.958820000
6	4.448935000	-0.520773000	-2.344712000
6	5.498847000	-0.300935000	-1.377206000
6	8.603610000	-2.620782000	1.248778000
6	9.358126000	-2.057903000	2.285729000
6	9.456439000	-0.675772000	2.496767000
6	10.413346000	0.830914000	-1.439370000
6	10.133675000	2.198962000	-1.322853000
6	8.932935000	2.689164000	-0.793359000
1	3.486398000	0.318289000	1.407067000
1	9.856744000	-2.723510000	2.981929000
1	10.860554000	2.909658000	-1.700805000
1	2.376218000	-0.560183000	-2.706253000
1	4.730333000	-0.730949000	-3.371489000
1	8.790554000	3.782077000	-0.801195000
1	11.362345000	0.549806000	-1.923794000
1	8.551521000	-3.720810000	1.206400000
1	10.032711000	-0.340397000	3.374172000
27	-7.983588000	-0.018394000	-0.025485000
8	-6.717384000	0.351937000	1.639427000
8	-6.048563000	-0.152345000	-0.849129000
8	-7.967012000	-1.970565000	0.542351000
8	-8.929592000	-0.562300000	-1.727588000
8	-9.685027000	0.341535000	1.005585000

8	-7.965201000	1.941978000	-0.576637000
6	-5.108152000	0.012541000	-0.039935000
6	-3.727795000	-0.046648000	-0.377449000
6	-2.759854000	0.198364000	0.579280000
6	-3.157477000	0.502458000	1.954748000
6	-4.454837000	0.571619000	2.341100000
6	-5.503228000	0.329193000	1.377190000
6	-8.610319000	-2.912503000	-0.005738000
6	-9.350767000	-2.849144000	-1.192878000
6	-9.442757000	-1.690762000	-1.976547000
6	-10.411940000	1.373814000	0.929866000
6	-10.123491000	2.556092000	0.235522000
6	-8.918575000	2.763604000	-0.448543000
1	-3.486960000	-0.242397000	-1.414564000
1	-9.844303000	-3.749518000	-1.542313000
1	-10.846424000	3.363947000	0.266748000
1	-2.382382000	0.626925000	2.702300000
1	-4.737291000	0.774034000	3.369146000
1	-8.768895000	3.752127000	-0.912536000
1	-11.363568000	1.334112000	1.484047000
1	-8.563955000	-3.888151000	0.504716000
1	-10.009771000	-1.764415000	-2.918631000

16 (R = CF₃; R₁= R₂= H; X = none)

E= -7288.79252 a.u., E_{ZPE}= -7288.37197 a.u.

27	5.683295000	0.086322000	0.141214000
8	5.856059000	1.912929000	-0.361847000
8	6.724883000	-0.579683000	-1.305857000
8	7.274078000	0.285331000	1.165772000
8	5.377616000	-1.716580000	0.662821000
6	6.491037000	2.305301000	-1.379042000
6	7.185520000	1.537626000	-2.315678000
6	7.243881000	0.148199000	-2.196829000
6	7.763309000	-0.622493000	1.893751000
6	7.282465000	-1.917019000	2.096542000
6	6.121831000	-2.355414000	1.456666000
1	7.684577000	2.024624000	-3.139444000
1	7.815151000	-2.587820000	2.753211000
6	6.442263000	3.840152000	-1.549078000
9	7.121660000	4.252703000	-2.637712000
9	5.165867000	4.249479000	-1.680528000
9	6.970218000	4.449302000	-0.475244000
6	8.020528000	-0.669784000	-3.252252000
9	8.613661000	0.118702000	-4.170478000
9	8.977098000	-1.406086000	-2.659430000
9	7.187647000	-1.503667000	-3.899173000
6	9.051745000	-0.171506000	2.616682000
9	9.971774000	0.228184000	1.720658000
9	8.788224000	0.859529000	3.438039000
9	9.593680000	-1.161178000	3.353761000
6	5.612716000	-3.791008000	1.715344000
9	5.499638000	-4.466039000	0.560672000

9	6.437544000	-4.484593000	2.524700000
9	4.399873000	-3.750027000	2.300021000
8	4.592086000	0.640787000	1.593191000
8	4.082131000	0.002732000	-0.876837000
6	3.064876000	0.329240000	-0.146928000
6	1.734457000	0.347807000	-0.623252000
6	0.700875000	0.693063000	0.234479000
6	1.002157000	1.042439000	1.596986000
6	2.283567000	1.046043000	2.091018000
6	3.350977000	0.684181000	1.234444000
1	1.557330000	0.049915000	-1.650785000
1	0.187015000	1.341045000	2.247476000
1	2.501780000	1.327157000	3.115683000
27	-5.683238000	0.086186000	-0.141042000
8	-5.377539000	-1.716672000	-0.662857000
8	-7.274072000	0.285155000	-1.165602000
8	-6.724790000	-0.579779000	1.306019000
8	-5.856127000	1.912838000	0.361741000
6	-6.121734000	-2.355486000	-1.456726000
6	-7.282433000	-1.917128000	-2.096514000
6	-7.763307000	-0.622627000	-1.893624000
6	-7.243847000	0.148179000	2.196903000
6	-7.185569000	1.537620000	2.315604000
6	-6.491168000	2.305263000	1.378883000
1	-7.815108000	-2.587911000	-2.753208000
1	-7.684674000	2.024666000	3.139313000
6	-5.612498000	-3.791007000	-1.715588000
9	-6.437325000	-4.484595000	-2.524944000
9	-4.399709000	-3.749849000	-2.300358000
9	-5.499259000	-4.466144000	-0.560990000
6	-9.051777000	-0.171628000	-2.616483000
9	-9.593693000	-1.161259000	-3.353634000
9	-9.971802000	0.227943000	-1.720395000
9	-8.788328000	0.859490000	-3.437753000
6	-8.020468000	-0.669739000	3.252397000
9	-8.976986000	-1.406151000	2.659632000
9	-7.187549000	-1.503514000	3.899413000
9	-8.613655000	0.118804000	4.170535000
6	-6.442606000	3.840143000	1.548708000
9	-6.970673000	4.449068000	0.474806000
9	-7.122032000	4.252744000	2.637304000
9	-5.166263000	4.249668000	1.680072000
8	-4.082087000	0.002655000	0.876944000
8	-4.592049000	0.640652000	-1.593098000
6	-3.350951000	0.684085000	-1.234352000
6	-2.283541000	1.045957000	-2.090931000
6	-1.002134000	1.042390000	-1.596900000
6	-0.700844000	0.693043000	-0.234386000
6	-1.734421000	0.347778000	0.623351000
6	-3.064832000	0.329177000	0.147025000
1	-2.501761000	1.327047000	-3.115601000
1	-0.186997000	1.341003000	-2.247393000

1	-1.557286000	0.049906000	1.650889000
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17 (R = CF₃; R₁ = R₂ = H; X = none)

E = -7288.78439 a.u., E_{ZPE} = -7288.36779 a.u.

27	5.768282000	-0.028139000	-0.138682000
8	4.365299000	-0.488658000	-1.684979000
8	3.926342000	0.105827000	0.832776000
8	5.888959000	-2.031718000	0.201180000
8	6.897847000	0.234321000	1.525077000
8	7.391460000	-0.071170000	-1.359935000
8	5.659284000	1.966799000	-0.515519000
6	2.922485000	-0.154647000	0.137958000
6	1.581039000	-0.167536000	0.621238000
6	0.530282000	-0.431543000	-0.234062000
6	0.803456000	-0.710378000	-1.649918000
6	2.049607000	-0.735835000	-2.176821000
6	3.183425000	-0.468418000	-1.319753000
6	6.664551000	-2.613456000	1.003077000
6	7.515154000	-2.033991000	1.951479000
6	7.544402000	-0.647036000	2.146926000
6	8.040233000	0.911973000	-1.799045000
6	7.719547000	2.271428000	-1.686260000
6	6.534583000	2.683864000	-1.067054000
1	1.432201000	0.084055000	1.664928000
1	8.128610000	-2.669420000	2.572354000
1	8.377469000	3.009947000	-2.119085000
1	-0.038754000	-0.945577000	-2.290990000
1	2.234924000	-0.971000000	-3.219692000
6	6.594733000	-4.155015000	0.912383000
9	5.353879000	-4.580972000	1.241993000
9	6.851551000	-4.570881000	-0.340558000
9	7.466899000	-4.771770000	1.737349000
6	8.438688000	-0.076568000	3.272343000
9	9.188007000	-1.024760000	3.875826000
9	9.276864000	0.855165000	2.781528000
9	7.679084000	0.507055000	4.221896000
6	6.185326000	4.189733000	-1.062387000
9	5.986098000	4.628186000	0.193676000
9	7.149855000	4.954406000	-1.616535000
9	5.046877000	4.403428000	-1.759513000
6	9.318892000	0.512474000	-2.571672000
9	10.110469000	-0.260155000	-1.804401000
9	8.996568000	-0.191014000	-3.676141000
9	10.046543000	1.579844000	-2.966251000
27	-5.867487000	-0.054191000	0.150749000
8	-5.944573000	-1.918962000	-0.206826000
8	-6.949728000	0.443940000	-1.323152000
8	-7.435320000	-0.255692000	1.202835000
8	-5.651218000	1.794680000	0.531765000
6	-6.579828000	-2.423739000	-1.173909000
6	-7.331141000	-1.767252000	-2.150020000
6	-7.451785000	-0.377396000	-2.141559000

6	-7.996792000	0.690282000	1.824210000
6	-7.602596000	2.026814000	1.895944000
6	-6.450535000	2.466287000	1.242026000
1	-7.823452000	-2.341245000	-2.920245000
1	-8.190692000	2.727061000	2.469463000
6	-6.452904000	-3.962855000	-1.224574000
9	-7.140234000	-4.493929000	-2.253737000
9	-5.159632000	-4.311994000	-1.366624000
9	-6.913802000	-4.509037000	-0.088717000
6	-8.285071000	0.318950000	-3.240402000
9	-8.857225000	-0.566748000	-4.078296000
9	-9.262109000	1.056003000	-2.684185000
9	-7.502890000	1.134321000	-3.968144000
6	-9.267086000	0.231696000	2.574558000
9	-10.143374000	-0.310956000	1.710856000
9	-8.953059000	-0.695070000	3.495629000
9	-9.880212000	1.252891000	3.202846000
6	-6.024497000	3.946110000	1.369671000
9	-5.940405000	4.515797000	0.157470000
9	-6.893700000	4.661214000	2.108874000
9	-4.816158000	4.025367000	1.958788000
8	-4.722142000	-0.445477000	1.628184000
8	-4.276569000	0.030485000	-0.889033000
6	-3.237111000	-0.200148000	-0.155735000
6	-1.917478000	-0.203961000	-0.639063000
6	-0.855285000	-0.443153000	0.231883000
6	-1.134532000	-0.705471000	1.626864000
6	-2.404232000	-0.726104000	2.131686000
6	-3.496681000	-0.464301000	1.258139000
1	-1.768126000	0.030220000	-1.686434000
1	-0.306730000	-0.931833000	2.289121000
1	-2.606235000	-0.946650000	3.174232000

18 (R = CF₃; R₁= R₂= H; X = none)

E= -7288.76617 a.u., E_{ZPE}= -7288.35331 a.u.

27	5.939080000	-0.012086000	-0.160755000
8	4.533941000	-0.460603000	-1.682147000
8	4.080263000	0.162587000	0.825064000
8	6.003019000	-2.004791000	0.206568000
8	7.066843000	0.234049000	1.500423000
8	7.547521000	-0.079116000	-1.382556000
8	5.859395000	1.976661000	-0.522101000
6	3.086011000	-0.112816000	0.131572000
6	1.735204000	-0.128825000	0.619058000
6	0.698097000	-0.412190000	-0.234688000
6	0.971672000	-0.713852000	-1.643814000
6	2.219072000	-0.736702000	-2.171845000
6	3.349173000	-0.447503000	-1.321203000
6	6.754905000	-2.605214000	1.019847000
6	7.617663000	-2.041968000	1.965242000
6	7.686834000	-0.653610000	2.140824000
6	8.219467000	0.894435000	-1.811632000

6	7.924957000	2.258247000	-1.686998000
6	6.746931000	2.686376000	-1.065890000
1	1.585891000	0.130192000	1.661203000
1	8.208882000	-2.687378000	2.597375000
1	8.597174000	2.988084000	-2.112688000
1	0.129899000	-0.965238000	-2.279920000
1	2.403923000	-0.987269000	-3.211135000
6	6.633929000	-4.143956000	0.943652000
9	5.375136000	-4.522078000	1.262696000
9	6.890945000	-4.579582000	-0.301827000
9	7.474829000	-4.778287000	1.785609000
6	8.590767000	-0.090020000	3.261977000
9	9.315838000	-1.049151000	3.875523000
9	9.449014000	0.817055000	2.761970000
9	7.840067000	0.519360000	4.201577000
6	6.421090000	4.197091000	-1.046647000
9	6.230751000	4.624489000	0.214095000
9	7.397274000	4.949109000	-1.594883000
9	5.285439000	4.432853000	-1.739865000
6	9.492926000	0.473891000	-2.581294000
9	10.270848000	-0.306149000	-1.807946000
9	9.161148000	-0.229050000	-3.682092000
9	10.233817000	1.530252000	-2.977187000
27	-5.939084000	-0.012104000	0.160798000
8	-4.080251000	0.162600000	-0.825039000
8	-4.533958000	-0.460619000	1.682158000
8	-5.859424000	1.976652000	0.522110000
8	-7.547514000	-0.079152000	1.382597000
8	-7.066856000	0.234042000	-1.500382000
8	-6.002979000	-2.004800000	-0.206588000
6	-3.349183000	-0.447512000	1.321229000
6	-2.219092000	-0.736718000	2.171879000
6	-0.971686000	-0.713863000	1.643861000
6	-0.698097000	-0.412186000	0.234741000
6	-1.735196000	-0.128817000	-0.619012000
6	-3.086008000	-0.112813000	-0.131540000
6	-6.746978000	2.686355000	1.065883000
6	-7.925002000	2.258210000	1.686987000
6	-8.219485000	0.894396000	1.811646000
6	-7.686816000	-0.653614000	-2.140816000
6	-7.617611000	-2.041976000	-1.965271000
6	-6.754845000	-2.605223000	-1.019885000
1	-2.403954000	-0.987296000	3.211165000
1	-8.597238000	2.988042000	2.112656000
1	-8.208811000	-2.687383000	-2.597424000
1	-0.129921000	-0.965257000	2.279974000
1	-1.585873000	0.130205000	-1.661155000
6	-6.421169000	4.197076000	1.046621000
9	-5.285536000	4.432872000	1.739858000
9	-6.230815000	4.624458000	-0.214123000
9	-7.397378000	4.949083000	1.594828000
6	-9.492947000	0.473841000	2.581295000

9	-10.233856000	1.530195000	2.977173000
9	-10.270850000	-0.306214000	1.807941000
9	-9.161174000	-0.229090000	3.682101000
6	-6.633835000	-4.143963000	-0.943723000
9	-6.890850000	-4.579622000	0.301745000
9	-7.474715000	-4.778294000	-1.785699000
9	-5.375031000	-4.522050000	-1.262767000
6	-8.590754000	-0.090016000	-3.261961000
9	-9.449012000	0.817042000	-2.761943000
9	-7.840057000	0.519386000	-4.201550000
9	-9.315812000	-1.049146000	-3.875523000

19 (R = CF₃; R₁= R₂= H; X= HC=CH)

E= -7366.16828 a.u., E_{ZPE}= -7365.71477 a.u.

27	6.949748000	0.000870000	0.115211000
8	6.893093000	1.902250000	0.087686000
8	8.070268000	-0.152014000	-1.416536000
8	8.500930000	0.135150000	1.213002000
8	6.879643000	-1.899752000	0.166262000
6	7.489500000	2.610750000	-0.768754000
6	8.283578000	2.191669000	-1.837884000
6	8.505880000	0.834046000	-2.072852000
6	9.111880000	-0.857520000	1.696749000
6	8.810830000	-2.211829000	1.544569000
6	7.710873000	-2.617886000	0.786669000
1	8.731394000	2.926167000	-2.489616000
1	9.434298000	-2.953799000	2.019528000
6	7.253006000	4.122059000	-0.552399000
9	7.934100000	4.875094000	-1.439060000
9	5.943535000	4.407820000	-0.689928000
9	7.634750000	4.487429000	0.681661000
6	9.387655000	0.408216000	-3.267337000
9	9.866785000	1.467926000	-3.949048000
9	10.437373000	-0.314170000	-2.835429000
9	8.680028000	-0.348605000	-4.123585000
6	10.327731000	-0.445025000	2.555427000
9	11.171740000	0.314548000	1.834930000
9	9.923281000	0.269514000	3.620464000
9	11.015278000	-1.511988000	3.009348000
6	7.407025000	-4.126309000	0.647195000
9	7.470690000	-4.499016000	-0.642186000
9	8.276886000	-4.886101000	1.342462000
9	6.169324000	-4.395454000	1.102392000
8	5.792884000	0.040708000	1.620829000
8	5.378204000	-0.017498000	-0.946804000
6	4.322672000	0.006391000	-0.194200000
6	3.003497000	0.003524000	-0.686991000
6	1.926541000	0.030860000	0.195460000
6	2.182158000	0.064846000	1.613524000
6	3.452811000	0.069877000	2.127898000
6	4.558684000	0.040187000	1.240242000
1	1.344141000	0.090674000	2.301168000

27	-6.949730000	0.001424000	-0.117110000
8	-6.878940000	-1.899195000	-0.167130000
8	-8.502173000	0.134419000	-1.213337000
8	-8.069079000	-0.150945000	1.415534000
8	-6.893676000	1.902834000	-0.090742000
6	-7.713232000	-2.618205000	-0.782396000
6	-8.816545000	-2.213219000	-1.535971000
6	-9.116300000	-0.859001000	-1.691501000
6	-8.503372000	0.835325000	2.072438000
6	-8.280801000	2.192834000	1.837164000
6	-7.488361000	2.611588000	0.766664000
1	-9.443127000	-2.955918000	-2.005663000
1	-8.727403000	2.927533000	2.489502000
6	-7.405153000	-4.126129000	-0.647108000
9	-8.303189000	-4.888979000	-1.301921000
9	-6.187322000	-4.397198000	-1.153631000
9	-7.413579000	-4.493145000	0.644889000
6	-10.335092000	-0.447609000	-2.546518000
9	-11.023191000	-1.515150000	-2.998213000
9	-11.177488000	0.311189000	-1.823141000
9	-9.934821000	0.267350000	-3.612741000
6	-9.383723000	0.409860000	3.268090000
9	-10.433774000	-0.312954000	2.837716000
9	-8.674945000	-0.346461000	4.123858000
9	-9.862283000	1.469751000	3.949894000
6	-7.251503000	4.122802000	0.550026000
9	-7.632492000	4.488091000	-0.684220000
9	-7.932764000	4.876169000	1.436272000
9	-5.941949000	4.408181000	0.688179000
8	-5.377711000	-0.015877000	0.944025000
8	-5.793609000	0.040809000	-1.623419000
6	-4.559233000	0.040501000	-1.243448000
6	-3.453711000	0.069637000	-2.131608000
6	-2.182819000	0.064765000	-1.617793000
6	-1.926603000	0.031468000	-0.199823000
6	-3.003182000	0.004811000	0.683110000
6	-4.322536000	0.007537000	0.190900000
1	-1.345069000	0.090183000	-2.305789000
6	0.580594000	0.027878000	-0.352587000
1	0.540188000	0.022630000	-1.439337000
6	-0.580531000	0.028404000	0.347856000
1	-0.540014000	0.023985000	1.434601000
1	-3.640469000	0.097723000	-3.199828000
1	-2.850400000	-0.021091000	1.757527000
1	2.851169000	-0.022913000	-1.761461000
1	3.639104000	0.098582000	3.196184000

20 (R = CF₃; R₁= R₂= H; X= HC=CH)

E= -7366.16295 a.u., E_{ZPE}= -7365.71328 a.u.

27	-7.019065000	0.010266000	0.094981000
8	-5.565988000	-0.079873000	1.668335000
8	-5.207131000	0.062908000	-0.928985000

8	-7.044892000	-2.028033000	0.137657000
8	-8.180842000	-0.093872000	-1.565625000
8	-8.626516000	0.114832000	1.339872000
8	-7.000214000	2.048460000	0.119546000
6	-4.175469000	0.021439000	-0.223230000
6	-2.844023000	0.026718000	-0.719324000
6	-1.764162000	-0.001055000	0.149788000
6	-1.998090000	-0.042117000	1.598359000
6	-3.235680000	-0.058860000	2.142640000
6	-4.394644000	-0.040961000	1.273439000
6	-7.788887000	-2.784534000	-0.537339000
6	-8.671648000	-2.432434000	-1.565380000
6	-8.780523000	-1.107315000	-2.006401000
6	-9.300732000	1.132679000	1.636532000
6	-9.032915000	2.467431000	1.303299000
6	-7.884324000	2.814247000	0.583694000
1	-9.249437000	-3.202001000	-2.054654000
1	-9.704502000	3.243400000	1.638424000
1	-1.139065000	-0.062868000	2.259703000
6	-7.639333000	-4.278864000	-0.169760000
9	-6.377227000	-4.694315000	-0.422715000
9	-7.880200000	-4.474616000	1.139187000
9	-8.475328000	-5.079085000	-0.865186000
6	-9.719042000	-0.798041000	-3.196133000
9	-10.388381000	-1.887784000	-3.632191000
9	-10.632200000	0.128107000	-2.846500000
9	-9.013053000	-0.311525000	-4.236970000
6	-7.593459000	4.311257000	0.330251000
9	-7.436212000	4.551365000	-0.983997000
9	-8.574313000	5.122021000	0.781320000
9	-6.449414000	4.673501000	0.954493000
6	-10.552234000	0.817595000	2.488952000
9	-11.357798000	-0.043969000	1.838284000
9	-10.194301000	0.248734000	3.657453000
9	-11.280105000	1.918683000	2.777807000
6	-0.434544000	0.009665000	-0.389798000
1	-0.388302000	0.031795000	-1.475479000
6	0.735461000	-0.005009000	0.321679000
1	0.687607000	-0.022029000	1.407512000
27	7.094253000	-0.004999000	-0.129512000
8	7.031318000	1.895464000	-0.116956000
8	8.642164000	-0.107714000	-1.230261000
8	8.214263000	0.088491000	1.397125000
8	7.023662000	-1.903635000	-0.171838000
6	7.886470000	2.632313000	-0.682177000
6	9.000065000	2.247560000	-1.430545000
6	9.280887000	0.898192000	-1.648823000
6	8.647719000	-0.922814000	2.017839000
6	8.417811000	-2.269842000	1.737004000
6	7.618145000	-2.647060000	0.656791000
1	9.645736000	3.002465000	-1.852764000
1	8.863644000	-3.028938000	2.361525000

6	7.584771000	4.136115000	-0.495117000
9	8.533177000	4.915963000	-1.048569000
9	6.407437000	4.442686000	-1.074713000
9	7.502898000	4.441361000	0.808970000
6	10.506939000	0.507543000	-2.503554000
9	11.204695000	1.585196000	-2.911460000
9	11.335192000	-0.278783000	-1.793618000
9	10.114281000	-0.170388000	-3.595721000
6	9.536605000	-0.539662000	3.221671000
9	10.590548000	0.185161000	2.805617000
9	8.837368000	0.198323000	4.100150000
9	10.006898000	-1.623081000	3.869323000
6	7.370146000	-4.148117000	0.387617000
9	7.746738000	-4.471241000	-0.859220000
9	8.046309000	-4.935213000	1.246250000
9	6.058156000	-4.426411000	0.517429000
8	5.522522000	-0.015066000	0.935510000
8	5.917864000	0.013033000	-1.633552000
6	4.696311000	0.007780000	-1.251865000
6	3.587987000	0.016611000	-2.148734000
6	2.322204000	0.013355000	-1.637968000
6	2.067927000	0.000368000	-0.213222000
6	3.148864000	-0.009813000	0.676211000
6	4.462030000	-0.005924000	0.191028000
1	1.483970000	0.019451000	-2.325417000
1	-2.700323000	0.061736000	-1.794919000
1	-3.399826000	-0.094139000	3.214653000
1	2.989569000	-0.018141000	1.749892000
1	3.780891000	0.024215000	-3.216101000

21 (R = CF₃; R₁= R₂= H; X= HC=CH)

E= -7366.14627 a.u., E_{ZPE}= -7365.70014 a.u.

27	7.186475000	-0.023047000	0.120865000
8	5.733097000	-0.092629000	1.682309000
8	5.348100000	-0.050100000	-0.916043000
8	7.136657000	1.996000000	0.320876000
8	8.339243000	0.254026000	-1.521381000
8	8.787568000	-0.202455000	1.350804000
8	7.214203000	-2.044831000	-0.054220000
6	4.329983000	-0.073657000	-0.202692000
6	2.985339000	-0.071275000	-0.694409000
6	1.922631000	-0.109705000	0.180460000
6	2.165099000	-0.153392000	1.628264000
6	3.404676000	-0.158248000	2.169338000
6	4.558906000	-0.110190000	1.296892000
6	7.867671000	2.831402000	-0.273857000
6	8.770314000	2.594340000	-1.315857000
6	8.916150000	1.315840000	-1.870331000
6	9.508703000	-1.219020000	1.517666000
6	9.289052000	-2.514824000	1.031545000
6	8.137410000	-2.824591000	0.300868000
1	9.333227000	3.418031000	-1.728506000

1	9.999234000	-3.294956000	1.261012000
1	1.309030000	-0.186591000	2.293054000
6	7.670265000	4.281205000	0.224136000
9	6.397885000	4.678586000	-0.004433000
9	7.894357000	4.363466000	1.547558000
9	8.487215000	5.162784000	-0.388202000
6	9.868863000	1.133424000	-3.074799000
9	10.504145000	2.275457000	-3.414482000
9	10.808202000	0.210793000	-2.792970000
9	9.182039000	0.711306000	-4.154868000
6	7.893116000	-4.292980000	-0.114858000
9	7.728601000	-4.389289000	-1.446458000
9	8.905203000	-5.113125000	0.235824000
9	6.768878000	-4.758591000	0.474506000
6	10.751272000	-0.958577000	2.400981000
9	11.457811000	0.082579000	1.925682000
9	10.371570000	-0.663568000	3.661382000
9	11.578659000	-2.023908000	2.462244000
27	-7.186279000	-0.023041000	-0.119774000
8	-5.348101000	-0.049871000	0.916786000
8	-5.733141000	-0.092516000	-1.681474000
8	-7.213905000	-2.044811000	0.055588000
8	-8.787122000	-0.202823000	-1.350077000
8	-8.339367000	0.254090000	1.522223000
8	-7.137104000	1.995938000	-0.320305000
6	-4.558914000	-0.110043000	-1.296121000
6	-3.404703000	-0.158074000	-2.168588000
6	-2.165121000	-0.153179000	-1.627530000
6	-1.922638000	-0.109503000	-0.179720000
6	-2.985335000	-0.071058000	0.695164000
6	-4.329962000	-0.073443000	0.203414000
6	-8.136314000	-2.824981000	-0.300656000
6	-9.287540000	-2.515603000	-1.032147000
6	-9.507566000	-1.219714000	-1.517883000
6	-8.917104000	1.315705000	1.870424000
6	-8.771823000	2.594041000	1.315436000
6	-7.868877000	2.831185000	0.273716000
1	-9.997048000	-3.296068000	-1.262562000
1	-9.335457000	3.417560000	1.727442000
1	-1.309014000	-0.186330000	-2.292280000
6	-7.891488000	-4.293395000	0.114675000
9	-6.766793000	-4.758266000	-0.474624000
9	-7.727274000	-4.390135000	1.446199000
9	-8.903046000	-5.113897000	-0.236653000
6	-10.749671000	-0.959601000	-2.401952000
9	-11.576542000	-2.025291000	-2.464006000
9	-11.456989000	0.081136000	-1.926885000
9	-10.369262000	-0.664144000	-3.662025000
6	-7.672103000	4.280883000	-0.224826000
9	-7.895832000	4.362416000	-1.548408000
9	-8.489826000	5.162238000	0.386824000
9	-6.400102000	4.679104000	0.003962000

6	-9.870376000	1.133201000	3.074436000
9	-10.809623000	0.210651000	2.792003000
9	-9.184118000	0.710900000	4.154788000
9	-10.505772000	2.275215000	3.413949000
6	0.578235000	-0.110662000	-0.357044000
1	0.532306000	-0.104433000	-1.442730000
6	-0.578271000	-0.110546000	0.357746000
1	-0.532290000	-0.104191000	1.443427000
1	-2.838250000	-0.042601000	1.770500000
1	-3.571484000	-0.190388000	-3.240216000
1	3.571464000	-0.190571000	3.240965000
1	2.838205000	-0.042817000	-1.769738000

22(R = CF₃; R₁= R₂= H; X= H₂C-CH₂)

E= -7367.38282 a.u., E_{ZPE}= -7366.90605 a.u.

27	-6.796101000	0.036065000	0.140444000
8	-6.548536000	-1.850005000	0.192948000
8	-7.857187000	0.015137000	-1.441323000
8	-8.376224000	-0.210087000	1.177455000
8	-6.914495000	1.934233000	0.114332000
6	-7.018163000	-2.645552000	-0.665866000
6	-7.791497000	-2.348998000	-1.789614000
6	-8.147524000	-1.031642000	-2.083193000
6	-9.093352000	0.735724000	1.605781000
6	-8.911090000	2.107302000	1.421315000
6	-7.828490000	2.590747000	0.684460000
1	-8.119806000	-3.147707000	-2.436960000
1	-9.616676000	2.801551000	1.851315000
6	-6.652633000	-4.117232000	-0.370190000
9	-7.086444000	-4.952510000	-1.335564000
9	-5.317440000	-4.256489000	-0.274666000
9	-7.200136000	-4.509613000	0.792897000
6	-9.001892000	-0.740857000	-3.336746000
9	-9.343899000	-1.868250000	-3.992144000
9	-10.135075000	-0.103935000	-2.991262000
9	-8.322196000	0.043627000	-4.191455000
6	-10.306429000	0.238876000	2.422845000
9	-11.077511000	-0.564317000	1.667340000
9	-9.894102000	-0.460182000	3.494127000
9	-11.074324000	1.256304000	2.862052000
6	-7.653400000	4.116007000	0.512464000
9	-7.616234000	4.442539000	-0.789449000
9	-8.654939000	4.811351000	1.087288000
9	-6.497938000	4.513789000	1.079374000
8	-5.710208000	0.170978000	1.691012000
8	-5.188673000	0.178062000	-0.856602000
6	-4.171857000	0.299818000	-0.063846000
6	-2.837104000	0.437108000	-0.508050000
6	-1.817658000	0.558899000	0.415569000
6	-2.121685000	0.547338000	1.818758000
6	-3.404970000	0.419830000	2.292816000
6	-4.464902000	0.292410000	1.361442000

1	-1.302611000	0.654383000	2.525189000
27	6.790716000	-0.036916000	-0.143175000
8	6.538665000	1.848590000	-0.183496000
8	8.384021000	-0.007977000	-1.187664000
8	7.843455000	0.206626000	1.426013000
8	6.914104000	-1.935174000	-0.128806000
6	7.318859000	2.650703000	-0.766140000
6	8.481825000	2.362095000	-1.482450000
6	8.916208000	1.044416000	-1.636372000
6	8.339568000	-0.740642000	2.096249000
6	8.246189000	-2.111365000	1.850872000
6	7.535754000	-2.592977000	0.749675000
1	9.049750000	3.166786000	-1.923844000
1	8.730566000	-2.806845000	2.519013000
6	6.855858000	4.119185000	-0.640456000
9	7.716903000	4.976257000	-1.224379000
9	5.655153000	4.275564000	-1.231587000
9	6.735588000	4.467505000	0.650735000
6	10.195769000	0.760496000	-2.453707000
9	10.813640000	1.894178000	-2.841460000
9	11.067693000	0.043416000	-1.723695000
9	9.893255000	0.056293000	-3.559179000
6	9.136780000	-0.245869000	3.323164000
9	10.140211000	0.560360000	2.930998000
9	8.337564000	0.449786000	4.150246000
9	9.673871000	-1.264008000	4.024942000
6	7.444261000	-4.117882000	0.519084000
9	7.920429000	-4.440679000	-0.693962000
9	8.141903000	-4.814247000	1.438703000
9	6.159637000	-4.517931000	0.587295000
8	5.190534000	-0.181969000	0.865006000
8	5.695080000	-0.174701000	-1.686077000
6	4.452774000	-0.302652000	-1.348150000
6	3.387960000	-0.440136000	-2.272500000
6	2.107795000	-0.566807000	-1.790068000
6	1.811698000	-0.567487000	-0.385147000
6	2.836277000	-0.438532000	0.531824000
6	4.168454000	-0.304216000	0.078970000
1	1.284933000	-0.681741000	-2.490840000
6	-0.379806000	0.674581000	-0.025854000
6	0.376123000	-0.680940000	0.064179000
1	-0.338587000	1.044731000	-1.055469000
1	0.143357000	1.409237000	0.597882000
1	-0.150166000	-1.416922000	-0.555344000
1	0.339410000	-1.048519000	1.094891000
1	3.609588000	-0.448919000	-3.334334000
1	2.650229000	-0.442320000	1.601571000
1	-2.645302000	0.451305000	-1.576688000
1	-3.632260000	0.418489000	3.353492000

23 (R = CF₃; R₁= R₂ = H; X= H₂C-CH₂)

E= -7367.37296 a.u., E_{ZPE}= -7366.90004 a.u.

27	6.888526000	-0.038433000	0.139947000
8	5.436905000	-0.097675000	1.711772000
8	5.030022000	-0.245638000	-0.882515000
8	6.719760000	1.988621000	0.199147000
8	8.020817000	0.187373000	-1.530866000
8	8.505377000	-0.051658000	1.370637000
8	7.014242000	-2.069783000	0.098669000
6	4.024889000	-0.305320000	-0.163303000
6	2.674232000	-0.443985000	-0.644147000
6	1.641525000	-0.513012000	0.241153000
6	1.890731000	-0.444299000	1.686292000
6	3.124568000	-0.317987000	2.228593000
6	4.266361000	-0.230769000	1.343570000
6	7.405067000	2.816857000	-0.456103000
6	8.319958000	2.557591000	-1.482384000
6	8.536061000	1.254208000	-1.950789000
6	9.277042000	-1.019002000	1.590994000
6	9.121454000	-2.352855000	1.189212000
6	7.981843000	-2.771479000	0.494156000
1	2.521790000	-0.503464000	-1.717578000
1	8.836720000	3.381032000	-1.952033000
1	9.873335000	-3.078370000	1.461045000
1	1.025828000	-0.512670000	2.341699000
1	3.295266000	-0.277628000	3.299296000
6	7.130239000	4.286002000	-0.062021000
9	5.838294000	4.599278000	-0.313788000
9	7.348362000	4.475496000	1.251859000
9	7.898751000	5.166075000	-0.737422000
6	9.489441000	1.047899000	-3.151116000
9	10.102289000	2.188907000	-3.535075000
9	10.447419000	0.153662000	-2.843863000
9	8.806434000	0.575500000	-4.214326000
6	7.815265000	-4.275867000	0.180870000
9	7.649817000	-4.472075000	-1.139946000
9	8.871006000	-5.017451000	0.577263000
9	6.720061000	-4.760565000	0.809282000
6	10.508775000	-0.645678000	2.449024000
9	11.143808000	0.419999000	1.929466000
9	10.122508000	-0.328176000	3.703061000
9	11.404977000	-1.652327000	2.541957000
6	0.213950000	-0.637971000	-0.215151000
6	-0.553263000	0.713882000	-0.116692000
1	0.185175000	-0.999802000	-1.247057000
1	-0.305466000	-1.380598000	0.403059000
1	-0.046478000	1.448631000	-0.753459000
1	-0.502143000	1.092961000	0.909319000
27	-6.968757000	0.045836000	-0.168281000
8	-6.697884000	-1.836006000	-0.122894000
8	-8.581259000	-0.048021000	-1.174299000
8	-7.986403000	-0.131704000	1.429546000
8	-7.107346000	1.941062000	-0.241506000
6	-7.489611000	-2.674235000	-0.635958000

6	-8.674765000	-2.431738000	-1.332030000
6	-9.120349000	-1.126441000	-1.547857000
6	-8.476733000	0.842334000	2.065798000
6	-8.399697000	2.200613000	1.755303000
6	-7.716655000	2.635315000	0.617884000
1	-9.250348000	-3.262340000	-1.711257000
1	-8.875169000	2.923307000	2.400685000
6	-7.011604000	-4.130355000	-0.441882000
9	-7.881438000	-5.024093000	-0.951176000
9	-5.826450000	-4.311088000	-1.057717000
9	-6.851263000	-4.403505000	0.862889000
6	-10.424167000	-0.893393000	-2.343022000
9	-11.041891000	-2.049902000	-2.654432000
9	-11.280904000	-0.146246000	-1.625632000
9	-10.157474000	-0.244484000	-3.490376000
6	-9.241082000	0.397710000	3.332250000
9	-10.233272000	-0.448670000	3.003080000
9	-8.410491000	-0.236259000	4.178284000
9	-9.785873000	1.440548000	3.989236000
6	-7.647389000	4.147920000	0.310610000
9	-8.193755000	4.409167000	-0.887708000
9	-8.296746000	4.883903000	1.233937000
9	-6.363875000	4.555420000	0.286296000
8	-5.347208000	0.248917000	0.799727000
8	-5.901532000	0.120817000	-1.738698000
6	-4.655302000	0.268681000	-1.431583000
6	-3.608515000	0.370424000	-2.382082000
6	-2.319342000	0.519711000	-1.931712000
6	-1.996876000	0.578703000	-0.534341000
6	-3.001323000	0.488302000	0.408449000
6	-4.343126000	0.334709000	-0.011175000
1	-1.512172000	0.608036000	-2.654307000
1	-3.851152000	0.334823000	-3.438710000
1	-2.795123000	0.538876000	1.473343000

24 (R = CF₃; R₁= R₂= H; X= H₂C-CH₂)

E= -7367.36082 a.u., E_{ZPE}= -7366.89163 a.u.

27	-7.036788000	0.023251000	0.152089000
8	-5.599071000	0.164523000	1.719947000
8	-5.177123000	0.145445000	-0.873014000
8	-6.890092000	-1.994758000	0.335333000
8	-8.161021000	-0.294198000	-1.505678000
8	-8.655546000	0.124782000	1.369288000
8	-7.147568000	2.044417000	-0.018332000
6	-4.174595000	0.234761000	-0.152048000
6	-2.819148000	0.320445000	-0.634285000
6	-1.790387000	0.428231000	0.251458000
6	-2.046133000	0.459502000	1.694829000
6	-3.285721000	0.386309000	2.235800000
6	-4.423365000	0.258582000	1.351637000
6	-7.585927000	-2.855730000	-0.265244000
6	-8.496413000	-2.651074000	-1.307183000

6	-8.691873000	-1.377773000	-1.859395000
6	-9.422334000	1.108794000	1.527043000
6	-9.255227000	2.413820000	1.044243000
6	-8.110373000	2.778703000	0.328391000
1	-2.662341000	0.309176000	-1.708747000
1	-9.024680000	-3.495552000	-1.723663000
1	-10.002198000	3.160644000	1.267612000
1	-1.185147000	0.560562000	2.351214000
1	-3.462261000	0.418808000	3.305803000
6	-7.328345000	-4.299290000	0.223100000
9	-6.040558000	-4.643025000	-0.010891000
9	-7.544679000	-4.399761000	1.546571000
9	-8.109140000	-5.210784000	-0.392719000
6	-9.640293000	-1.233478000	-3.072505000
9	-10.251703000	-2.392735000	-3.398074000
9	-10.598457000	-0.324168000	-2.814092000
9	-8.952857000	-0.816904000	-4.155286000
6	-7.929158000	4.258433000	-0.079354000
9	-7.761375000	4.368130000	-1.409720000
9	-8.977880000	5.032489000	0.268657000
9	-6.829479000	4.770323000	0.518332000
6	-10.661834000	0.794338000	2.397170000
9	-11.312878000	-0.281648000	1.919932000
9	-10.283932000	0.523916000	3.663918000
9	-11.540002000	1.819233000	2.443071000
6	-0.358069000	0.507318000	-0.208599000
6	0.397202000	-0.838657000	-0.003383000
1	-0.326980000	0.793356000	-1.264249000
1	0.164269000	1.291380000	0.353429000
1	-0.109236000	-1.617585000	-0.586857000
1	0.343950000	-1.138053000	1.047730000
27	7.054239000	-0.117613000	-0.171456000
8	5.679678000	-0.369532000	-1.788387000
8	5.187499000	-0.409640000	0.792216000
8	7.448728000	-2.103215000	-0.293337000
8	8.142269000	-0.087415000	1.537519000
8	8.645575000	0.372590000	-1.331088000
8	6.627132000	1.871296000	-0.083496000
6	4.208448000	-0.518757000	0.042214000
6	2.845408000	-0.662936000	0.486583000
6	1.839388000	-0.742999000	-0.427690000
6	2.130839000	-0.713523000	-1.864320000
6	3.381456000	-0.593203000	-2.370743000
6	4.495583000	-0.484480000	-1.454263000
6	8.318746000	-2.736137000	0.361094000
6	9.093705000	-2.275858000	1.431341000
6	8.920744000	-0.985488000	1.949315000
6	9.137193000	1.517038000	-1.500591000
6	8.612192000	2.747981000	-1.082682000
6	7.379711000	2.821476000	-0.426299000
1	2.662027000	-0.690398000	1.556510000
1	9.804998000	-2.942459000	1.895510000

1	9.148216000	3.657127000	-1.310202000
1	1.288492000	-0.805237000	-2.545761000
1	3.584427000	-0.581418000	-3.436495000
6	8.474014000	-4.207138000	-0.087609000
9	7.321521000	-4.880164000	0.130944000
9	8.747553000	-4.277919000	-1.402237000
9	9.455052000	-4.856526000	0.573225000
6	9.729691000	-0.574001000	3.201384000
9	10.647669000	-1.497929000	3.556978000
9	10.377810000	0.584877000	2.985181000
9	8.901347000	-0.397004000	4.251999000
6	6.800006000	4.212980000	-0.086042000
9	6.574161000	4.323302000	1.236236000
9	7.611461000	5.226381000	-0.450883000
9	5.618200000	4.389343000	-0.720585000
6	10.464773000	1.507723000	-2.294310000
9	11.372463000	0.727140000	-1.678395000
9	10.265681000	1.016174000	-3.533360000
9	11.003597000	2.739212000	-2.424472000

MECP₂₂₋₂₃ (R = CF₃; R₁ = R₂ = H; X = H₂C-CH₂)

E = -7367.36611 a.u.

27	6.806649000	-0.035537000	0.146514000
8	5.527210000	-0.122667000	1.685205000
8	5.096742000	-0.178721000	-0.883591000
8	6.673906000	1.943456000	0.197118000
8	7.958240000	0.085518000	-1.465490000
8	8.419487000	0.044487000	1.301823000
8	6.942538000	-2.013570000	0.097833000
6	4.072383000	-0.263660000	-0.142871000
6	2.735916000	-0.382462000	-0.623228000
6	1.698156000	-0.497160000	0.267840000
6	1.959021000	-0.485447000	1.693675000
6	3.214549000	-0.374593000	2.216703000
6	4.322739000	-0.250448000	1.322000000
6	7.359155000	2.748036000	-0.488771000
6	8.266257000	2.454197000	-1.511142000
6	8.477920000	1.135571000	-1.927262000
6	9.190715000	-0.914686000	1.566346000
6	9.039025000	-2.261412000	1.218466000
6	7.907686000	-2.701226000	0.525126000
1	2.576187000	-0.399877000	-1.696973000
1	8.786538000	3.258844000	-2.008326000
1	9.790402000	-2.975763000	1.518618000
1	1.109724000	-0.582611000	2.365155000
1	3.403563000	-0.374985000	3.284847000
6	7.095905000	4.227458000	-0.126034000
9	5.806260000	4.541559000	-0.371563000
9	7.334172000	4.443891000	1.178674000
9	7.865920000	5.078784000	-0.834152000
6	9.439056000	0.869011000	-3.108442000
9	10.054451000	1.991027000	-3.536253000

9	10.391871000	-0.009643000	-2.746675000
9	8.764271000	0.347887000	-4.150959000
6	7.744609000	-4.211956000	0.241630000
9	7.606825000	-4.432942000	-1.076908000
9	8.796417000	-4.936711000	0.674967000
9	6.641173000	-4.681209000	0.860472000
6	10.419279000	-0.496172000	2.406818000
9	11.050476000	0.543581000	1.834068000
9	10.029976000	-0.120590000	3.641214000
9	11.313754000	-1.497073000	2.544996000
6	0.271462000	-0.621339000	-0.199071000
6	-0.507055000	0.722038000	-0.095607000
1	0.251455000	-0.974394000	-1.234780000
1	-0.248725000	-1.373499000	0.406114000
1	-0.005585000	1.465373000	-0.727204000
1	-0.459677000	1.094599000	0.932771000
27	-6.921603000	0.041976000	-0.166138000
8	-6.659814000	-1.840507000	-0.082733000
8	-8.530192000	-0.064412000	-1.178865000
8	-7.951329000	-0.103135000	1.428723000
8	-7.057538000	1.935948000	-0.277169000
6	-7.455241000	-2.684196000	-0.580393000
6	-8.637109000	-2.449800000	-1.285421000
6	-9.074651000	-1.147172000	-1.530701000
6	-8.453448000	0.882837000	2.036421000
6	-8.378150000	2.234043000	1.695897000
6	-7.681255000	2.646027000	0.558244000
1	-9.216477000	-3.285195000	-1.647988000
1	-8.864349000	2.969277000	2.318653000
6	-6.988024000	-4.139190000	-0.354117000
9	-7.865963000	-5.037517000	-0.842620000
9	-5.805435000	-4.343673000	-0.966901000
9	-6.828990000	-4.384849000	0.956120000
6	-10.376111000	-0.923122000	-2.331998000
9	-10.995105000	-2.082358000	-2.630566000
9	-11.234019000	-0.165939000	-1.625647000
9	-10.107119000	-0.288294000	-3.486816000
6	-9.233807000	0.463579000	3.301603000
9	-10.222229000	-0.389009000	2.976023000
9	-8.415516000	-0.153558000	4.171323000
9	-9.787646000	1.519259000	3.930729000
6	-7.614889000	4.151698000	0.218279000
9	-8.142792000	4.382850000	-0.994762000
9	-8.283939000	4.904905000	1.113528000
9	-6.333691000	4.566802000	0.205753000
8	-5.306391000	0.261854000	0.806186000
8	-5.847135000	0.082535000	-1.731308000
6	-4.601860000	0.239611000	-1.420864000
6	-3.550742000	0.322489000	-2.367907000
6	-2.264425000	0.485911000	-1.914076000
6	-1.948558000	0.577398000	-0.516639000
6	-2.958699000	0.504875000	0.422051000

6	-4.297255000	0.336619000	-0.001059000
1	-1.453398000	0.559152000	-2.633971000
1	-3.787864000	0.261562000	-3.424705000
1	-2.757242000	0.578571000	1.486399000

MECP₂₃₋₂₄ (R = CF₃; R₁= R₂ = H; X= H₂C-CH₂)

E= -7367.35524 a.u.

27	-6.963901000	0.021178000	0.161393000
8	-5.691379000	0.203699000	1.708695000
8	-5.230610000	0.067479000	-0.851514000
8	-6.855989000	-1.951987000	0.364195000
8	-8.087756000	-0.219659000	-1.455750000
8	-8.591140000	0.055812000	1.300768000
8	-7.075229000	1.991457000	-0.035190000
6	-4.215837000	0.191400000	-0.106619000
6	-2.871212000	0.262599000	-0.578361000
6	-1.842829000	0.420730000	0.315677000
6	-2.116538000	0.504911000	1.736254000
6	-3.379187000	0.445974000	2.250832000
6	-4.481660000	0.281790000	1.353665000
6	-7.545125000	-2.801431000	-0.262479000
6	-8.437575000	-2.578357000	-1.314953000
6	-8.619705000	-1.294207000	-1.840054000
6	-9.357287000	1.040067000	1.476786000
6	-9.183107000	2.353875000	1.029858000
6	-8.035269000	2.724819000	0.323701000
1	-2.702073000	0.210737000	-1.649628000
1	-8.964775000	-3.412373000	-1.752447000
1	-9.929719000	3.098320000	1.261877000
1	-1.273365000	0.636112000	2.410112000
1	-3.578436000	0.519231000	3.314661000
6	-7.301549000	-4.250834000	0.218287000
9	-6.015469000	-4.598525000	-0.000325000
9	-7.542675000	-4.358607000	1.535378000
9	-8.081708000	-5.145475000	-0.421173000
6	-9.559334000	-1.109553000	-3.053259000
9	-10.170241000	-2.257107000	-3.412825000
9	-10.515288000	-0.206031000	-2.768846000
9	-8.864636000	-0.662689000	-4.116818000
6	-7.842589000	4.207365000	-0.067381000
9	-7.677838000	4.327919000	-1.395638000
9	-8.889827000	4.977484000	0.291768000
9	-6.742664000	4.703725000	0.536172000
6	-10.607152000	0.698393000	2.321091000
9	-11.246185000	-0.365511000	1.803475000
9	-10.244651000	0.396020000	3.583245000
9	-11.485014000	1.720623000	2.378302000
6	-0.409496000	0.502717000	-0.146334000
6	0.349741000	-0.844512000	0.037091000
1	-0.380641000	0.801877000	-1.198873000
1	0.116637000	1.279254000	0.421785000
1	-0.158158000	-1.616872000	-0.554445000

1	0.300713000	-1.156205000	1.084627000
27	7.010140000	-0.109389000	-0.169342000
8	5.615067000	-0.320379000	-1.780698000
8	5.145351000	-0.414684000	0.803949000
8	7.389712000	-2.096345000	-0.336362000
8	8.117410000	-0.121796000	1.529337000
8	8.597686000	0.388221000	-1.333704000
8	6.603486000	1.882388000	-0.037703000
6	4.160124000	-0.512256000	0.061529000
6	2.801871000	-0.672859000	0.513267000
6	1.787757000	-0.738753000	-0.393620000
6	2.068212000	-0.674284000	-1.833041000
6	3.313294000	-0.537190000	-2.348066000
6	4.435097000	-0.445421000	-1.439289000
6	8.264629000	-2.746315000	0.293753000
6	9.054437000	-2.313562000	1.365130000
6	8.895315000	-1.032552000	1.911717000
6	9.100405000	1.530415000	-1.480573000
6	8.592874000	2.758118000	-1.031083000
6	7.365420000	2.830425000	-0.363736000
1	2.626691000	-0.724453000	1.583660000
1	9.768232000	-2.993232000	1.805897000
1	9.138228000	3.665955000	-1.240947000
1	1.219636000	-0.752372000	-2.508352000
1	3.506518000	-0.499114000	-3.415025000
6	8.409612000	-4.207119000	-0.189918000
9	7.256035000	-4.880759000	0.021774000
9	8.672787000	-4.248858000	-1.507943000
9	9.392992000	-4.876702000	0.447775000
6	9.723922000	-0.651928000	3.160468000
9	10.641027000	-1.588753000	3.485160000
9	10.377127000	0.506802000	2.959166000
9	8.911850000	-0.490899000	4.226423000
6	6.805594000	4.220838000	0.012078000
9	6.585691000	4.302932000	1.337358000
9	7.629731000	5.232297000	-0.331171000
9	5.624407000	4.429003000	-0.613857000
6	10.421531000	1.524552000	-2.284775000
9	11.324328000	0.717297000	-1.696796000
9	10.206908000	1.067485000	-3.534651000
9	10.975855000	2.752111000	-2.388435000

25 (R = CF₃; R₁= R₂= H; X= piperazindiyl)

E= -7555.43187 a.u., E_{ZPE}= -7554.88495 a.u.

7	1.393963000	-0.059392000	0.349064000
6	0.411645000	-0.855912000	1.090702000
6	-0.985084000	-0.238536000	1.031877000
7	-1.391768000	-0.021079000	-0.353931000
6	-0.409267000	0.774926000	-1.095974000
6	0.987445000	0.157954000	-1.036800000
1	0.709597000	-0.950049000	2.133929000
1	0.374346000	-1.872140000	0.665268000

1	-1.679558000	-0.935939000	1.503551000
1	-1.003518000	0.706564000	1.599506000
1	-0.707310000	0.868274000	-2.139291000
1	-0.372088000	1.791568000	-0.671334000
1	1.681354000	0.855814000	-1.508413000
1	1.006893000	-0.787095000	-1.604304000
27	-7.730678000	-0.002413000	-0.168514000
8	-7.682130000	-1.906334000	-0.197940000
8	-9.377927000	0.128506000	-1.129816000
8	-8.714703000	-0.123222000	1.461402000
8	-7.656224000	1.900155000	-0.171713000
6	-8.564156000	-2.623990000	-0.743186000
6	-9.719951000	-2.219831000	-1.414248000
6	-10.028994000	-0.865069000	-1.552559000
6	-9.052659000	0.873975000	2.155365000
6	-8.819642000	2.225534000	1.893973000
6	-8.137819000	2.623038000	0.742061000
1	-10.382509000	-2.963501000	-1.829834000
1	-9.175836000	2.972091000	2.587127000
6	-8.253471000	-4.132371000	-0.622771000
9	-9.213585000	-4.897688000	-1.180331000
9	-7.090814000	-4.417148000	-1.241890000
9	-8.138080000	-4.489235000	0.667253000
6	-11.313448000	-0.457381000	-2.307157000
9	-12.028708000	-1.526484000	-2.712751000
9	-12.103193000	0.290074000	-1.514855000
9	-11.004445000	0.268478000	-3.396404000
6	-9.813101000	0.474361000	3.438796000
9	-10.906187000	-0.246138000	3.129741000
9	-9.027089000	-0.275228000	4.232423000
9	-10.213672000	1.547985000	4.150170000
6	-7.903301000	4.128682000	0.488796000
9	-8.493278000	4.510937000	-0.656329000
9	-8.393546000	4.896135000	1.483652000
9	-6.584410000	4.383289000	0.386438000
8	-6.080385000	-0.021240000	0.754080000
8	-6.716588000	0.009011000	-1.769720000
6	-5.450185000	0.013215000	-1.494473000
6	-4.427418000	0.042015000	-2.472432000
6	-3.113020000	0.045638000	-2.077511000
6	-2.739639000	0.025321000	-0.686351000
6	-3.742059000	-0.006753000	0.291081000
6	-5.088619000	-0.014456000	-0.089446000
1	-2.342018000	0.014895000	-2.837653000
1	-4.703700000	0.042647000	-3.521503000
1	-3.521382000	0.011327000	1.350456000
27	7.732470000	-0.006490000	0.171955000
8	7.697427000	-1.910384000	0.133081000
8	9.380119000	0.101935000	1.135378000
8	8.716693000	-0.061418000	-1.461057000
8	7.644118000	1.894514000	0.243675000
6	8.585599000	-2.640850000	0.650712000

6	9.739713000	-2.252681000	1.333865000
6	10.039392000	-0.901519000	1.520291000
6	9.040873000	0.962065000	-2.122550000
6	8.793188000	2.301393000	-1.815639000
6	8.113501000	2.652689000	-0.647513000
1	10.408288000	-3.006022000	1.721446000
1	9.137720000	3.074804000	-2.484842000
6	8.285460000	-4.146145000	0.476826000
9	9.253776000	-4.923943000	1.002073000
9	7.127779000	-4.461902000	1.090533000
9	8.166535000	-4.456972000	-0.824577000
6	11.323445000	-0.512268000	2.285283000
9	12.045708000	-1.590414000	2.652761000
9	12.106937000	0.265877000	1.516656000
9	11.013387000	0.174644000	3.399187000
6	9.804187000	0.613555000	-3.419112000
9	10.916487000	-0.086924000	-3.132275000
9	9.033600000	-0.135527000	-4.227779000
9	10.174774000	1.714001000	-4.105234000
6	7.865190000	4.146520000	-0.342480000
9	8.458867000	4.496939000	0.810844000
9	8.340578000	4.951759000	-1.314539000
9	6.544442000	4.383513000	-0.223273000
8	6.083099000	-0.002540000	-0.751868000
8	6.717292000	-0.062489000	1.771858000
6	5.451081000	-0.067883000	1.495486000
6	4.427246000	-0.109387000	2.471914000
6	3.113250000	-0.120605000	2.075492000
6	2.741188000	-0.096862000	0.683989000
6	3.744937000	-0.050806000	-0.291822000
6	5.090624000	-0.030431000	0.090480000
1	2.341532000	-0.098542000	2.835169000
1	4.702116000	-0.110914000	3.521360000
1	3.526425000	-0.069159000	-1.351606000

26 (R = CF₃; R₁= R₂= H; X= piperazindiyl)

E= -7555.42782 a.u., E_{ZPE}= -7554.88452 a.u.

27	7.831673000	-0.000976000	0.163838000
8	6.463971000	-0.026387000	1.852033000
8	5.909095000	-0.077602000	-0.729403000
8	7.780445000	2.035472000	0.283487000
8	8.878979000	0.194809000	-1.573865000
8	9.522785000	-0.124896000	1.301750000
8	7.840970000	-2.048129000	0.103211000
6	4.938477000	-0.095780000	0.050372000
6	3.576692000	-0.154183000	-0.342889000
6	2.570840000	-0.227776000	0.605503000
6	2.913680000	-0.212746000	2.041511000
6	4.182738000	-0.151394000	2.490688000
6	5.277508000	-0.092226000	1.535176000
6	8.449483000	2.837944000	-0.417138000
6	9.270209000	2.553439000	-1.514429000

6	9.398325000	1.249618000	-2.015204000
6	10.244795000	-1.138454000	1.471009000
6	9.988642000	-2.457443000	1.070058000
6	8.788262000	-2.804011000	0.439281000
1	3.379596000	-0.199080000	-1.405923000
1	9.783093000	3.361921000	-2.013307000
1	10.711344000	-3.227584000	1.293880000
1	2.106719000	-0.197907000	2.764092000
1	4.421600000	-0.112884000	3.548480000
6	8.268974000	4.314613000	0.003696000
9	6.984337000	4.697855000	-0.189842000
9	8.550267000	4.479621000	1.308994000
9	9.051445000	5.165049000	-0.694773000
6	10.246353000	1.032693000	-3.290834000
9	10.871699000	2.157499000	-3.704803000
9	11.190956000	0.097092000	-3.079355000
9	9.463970000	0.608215000	-4.305893000
6	8.522323000	-4.294746000	0.127537000
9	8.288044000	-4.474075000	-1.186034000
9	9.549082000	-5.100901000	0.473366000
9	7.428678000	-4.723393000	0.800242000
6	11.541403000	-0.850206000	2.264208000
9	12.207331000	0.188617000	1.728951000
9	11.243923000	-0.535682000	3.544074000
9	12.385132000	-1.906074000	2.292832000
7	1.239342000	-0.245199000	0.273733000
6	0.240767000	-0.997467000	1.049112000
6	-1.144362000	-0.356696000	0.975820000
7	-1.551864000	-0.189025000	-0.414275000
6	-0.570545000	0.585889000	-1.176774000
6	0.821649000	-0.042071000	-1.116757000
1	0.541885000	-1.075494000	2.092351000
1	0.186146000	-2.019913000	0.645826000
1	-1.845358000	-1.025745000	1.478386000
1	-1.143808000	0.607658000	1.511475000
1	-0.871953000	0.658337000	-2.220991000
1	-0.521190000	1.612759000	-0.777779000
1	1.521114000	0.639663000	-1.602246000
1	0.833097000	-0.999072000	-1.660123000
27	-7.891509000	0.005465000	-0.180069000
8	-7.879358000	-1.896779000	-0.107755000
8	-9.543444000	0.118750000	-1.129092000
8	-8.860417000	-0.007214000	1.460236000
8	-7.776317000	1.902371000	-0.286204000
6	-8.783058000	-2.625399000	-0.601654000
6	-9.938673000	-2.233975000	-1.279770000
6	-10.221255000	-0.882508000	-1.488346000
6	-9.172995000	1.032624000	2.102483000
6	-8.915212000	2.363047000	1.767168000
6	-8.235433000	2.683908000	0.590588000
1	-10.621869000	-2.984712000	-1.646429000
1	-9.249897000	3.153150000	2.421794000

6	-8.501050000	-4.130851000	-0.400960000
9	-9.482327000	-4.905318000	-0.904776000
9	-7.351191000	-4.472232000	-1.015634000
9	-8.377196000	-4.417158000	0.905618000
6	-11.508162000	-0.488445000	-2.246346000
9	-12.245653000	-1.563202000	-2.590954000
9	-12.273868000	0.309301000	-1.480237000
9	-11.200359000	0.179118000	-3.372142000
6	-9.932264000	0.715971000	3.409683000
9	-11.054526000	0.024775000	3.141114000
9	-9.165179000	-0.028912000	4.225443000
9	-10.283834000	1.832558000	4.078371000
6	-7.970698000	4.168277000	0.254488000
9	-8.564203000	4.501598000	-0.903584000
9	-8.432256000	4.997759000	1.211798000
9	-6.647262000	4.385653000	0.125756000
8	-6.229658000	-0.001172000	0.728410000
8	-6.888577000	-0.089006000	-1.788859000
6	-5.621583000	-0.100474000	-1.524135000
6	-4.605863000	-0.147267000	-2.509943000
6	-3.289099000	-0.158575000	-2.123843000
6	-2.906729000	-0.117675000	-0.736389000
6	-3.896584000	-0.071632000	0.248550000
6	-5.248777000	-0.063838000	-0.121355000
1	-2.523540000	-0.248484000	-2.885441000
1	-4.890563000	-0.192963000	-3.555703000
1	-3.666723000	-0.005999000	1.304299000

27 (R = CF₃; R₁ = R₂ = H; X = piperazindiyil)

E = -7555.42129 a.u., E_{ZPE} = -7554.88159 a.u.

27	7.999758000	0.001993000	-0.180618000
8	6.646177000	-0.024679000	-1.874047000
8	6.067483000	0.003919000	0.701212000
8	8.015699000	-2.030696000	-0.327244000
8	9.033701000	-0.187553000	1.562319000
8	9.686631000	0.209348000	-1.303003000
8	7.928640000	2.042089000	-0.082572000
6	5.105170000	-0.011073000	-0.086392000
6	3.736793000	-0.037688000	0.298523000
6	2.740622000	-0.084000000	-0.657142000
6	3.091765000	-0.089643000	-2.089626000
6	4.365660000	-0.063111000	-2.530757000
6	5.454611000	-0.035054000	-1.568187000
6	8.704815000	-2.823585000	0.365823000
6	9.506711000	-2.529698000	1.473891000
6	9.585412000	-1.229918000	1.994872000
6	10.368072000	1.253463000	-1.458507000
6	10.056490000	2.555732000	-1.042914000
6	8.843940000	2.842514000	-0.405956000
1	3.530769000	-0.061880000	1.360828000
1	10.041671000	-3.328132000	1.965727000
1	10.745839000	3.358632000	-1.256630000

1	2.289089000	-0.060408000	-2.817112000
1	4.612503000	-0.041520000	-3.587173000
6	8.572500000	-4.297963000	-0.079364000
9	7.298814000	-4.722349000	0.101944000
9	8.864196000	-4.432792000	-1.385494000
9	9.377212000	-5.133932000	0.609882000
6	10.412859000	-1.001993000	3.281962000
9	11.057863000	-2.115286000	3.695288000
9	11.337813000	-0.043744000	3.087136000
9	9.608243000	-0.602356000	4.289276000
6	8.517161000	4.314785000	-0.066257000
9	8.284366000	4.459581000	1.251915000
9	9.506479000	5.168669000	-0.403594000
9	7.401661000	4.707802000	-0.724282000
6	11.686399000	1.020142000	-2.233135000
9	12.445959000	0.103197000	-1.603587000
9	11.426183000	0.560851000	-3.474302000
9	12.425539000	2.143911000	-2.361939000
27	-7.992829000	0.015053000	0.180081000
8	-6.639266000	0.075294000	1.870127000
8	-6.062293000	0.036908000	-0.704463000
8	-7.957746000	-2.013775000	0.374514000
8	-9.025541000	-0.240527000	-1.555334000
8	-9.684262000	0.199850000	1.300265000
8	-7.980357000	2.053048000	0.033551000
6	-5.099067000	0.051436000	0.082493000
6	-3.731056000	0.063802000	-0.303377000
6	-2.733862000	0.129140000	0.650776000
6	-3.085158000	0.160420000	2.082961000
6	-4.359061000	0.149366000	2.524737000
6	-5.447980000	0.097384000	1.563354000
6	-8.634124000	-2.837992000	-0.293960000
6	-9.448372000	-2.589103000	-1.404160000
6	-9.556698000	-1.305295000	-1.958200000
6	-10.400486000	1.225122000	1.420892000
6	-10.131101000	2.523217000	0.964743000
6	-8.923584000	2.831857000	0.328383000
1	-3.526505000	0.074367000	-1.366117000
1	-9.969742000	-3.410733000	-1.871810000
1	-10.848988000	3.308234000	1.149169000
1	-2.283226000	0.139469000	2.811400000
1	-4.605504000	0.145707000	3.581459000
6	-8.468005000	-4.297772000	0.186699000
9	-7.187615000	-4.701089000	0.003597000
9	-8.744821000	-4.405602000	1.498428000
9	-9.261892000	-5.166761000	-0.473720000
6	-10.393353000	-1.128579000	-3.247364000
9	-11.021087000	-2.264001000	-3.625682000
9	-11.333653000	-0.180905000	-3.076020000
9	-9.599656000	-0.744602000	-4.269386000
6	-8.641537000	4.304391000	-0.048179000
9	-8.402244000	4.421991000	-1.367801000

9	-9.660768000	5.134376000	0.258763000
9	-7.545089000	4.750330000	0.608023000
6	-11.704984000	0.978836000	2.214896000
9	-12.380375000	-0.067565000	1.706781000
9	-11.418566000	0.700291000	3.504960000
9	-12.534106000	2.045827000	2.204712000
7	-1.394729000	0.092261000	0.329736000
6	-0.392453000	0.866876000	1.074179000
6	0.983643000	0.202636000	1.043560000
7	1.401103000	-0.045416000	-0.336875000
6	0.400079000	-0.819559000	-1.083199000
6	-0.977798000	-0.159026000	-1.050574000
1	-0.696015000	0.995576000	2.111777000
1	-0.319051000	1.871002000	0.628833000
1	1.693639000	0.883815000	1.515000000
1	0.969047000	-0.736224000	1.618695000
1	0.704073000	-0.944629000	-2.121301000
1	0.329372000	-1.825237000	-0.640756000
1	-1.686168000	-0.843514000	-1.519441000
1	-0.967682000	0.778583000	-1.627722000

28 (R=H; R₁=CH₃; R₂=*tert*-C₄H₉; X=none)

E= -4985.81661 a.u., E_{ZPE}= -4985.15362 a.u.

27	5.661178000	0.507227000	-0.373138000
8	5.424994000	2.083273000	0.679717000
8	6.523184000	1.368987000	-1.833100000
8	7.343781000	0.289541000	0.486883000
8	5.748449000	-1.106098000	-1.392366000
6	5.811230000	3.229608000	0.305295000
6	6.446625000	3.565408000	-0.893221000
6	6.750877000	2.615797000	-1.870122000
6	8.112011000	-0.697480000	0.277284000
6	7.896708000	-1.774228000	-0.584517000
6	6.735563000	-1.897880000	-1.352762000
1	6.711652000	4.600703000	-1.070936000
1	8.655083000	-2.544470000	-0.657449000
8	4.744926000	-0.453692000	0.997995000
8	3.927816000	0.796969000	-1.111735000
6	3.010293000	0.246131000	-0.385765000
6	1.628675000	0.331922000	-0.727186000
6	0.735915000	-0.287447000	0.132472000
6	1.199307000	-0.974831000	1.306397000
6	2.522086000	-1.087807000	1.681123000
6	3.464916000	-0.456201000	0.806294000
1	0.434360000	-1.435064000	1.920857000
27	-5.658564000	0.528025000	0.349368000
8	-5.735412000	-1.026301000	1.457052000
8	-7.345870000	0.259728000	-0.486658000
8	-6.515382000	1.467405000	1.763634000
8	-5.431529000	2.043759000	-0.790644000
6	-6.720559000	-1.821488000	1.467280000
6	-7.886329000	-1.743511000	0.700024000

6	-8.109817000	-0.716400000	-0.218470000
6	-6.746449000	2.713745000	1.732345000
6	-6.449377000	3.608401000	0.702797000
6	-5.818877000	3.208205000	-0.478417000
1	-8.642036000	-2.510523000	0.819797000
1	-6.716417000	4.651294000	0.824114000
8	-3.921947000	0.860978000	1.061413000
8	-4.747536000	-0.505306000	-0.971676000
6	-3.466685000	-0.496428000	-0.786118000
6	-2.527159000	-1.175026000	-1.628915000
6	-1.202845000	-1.042484000	-1.265904000
6	-0.735102000	-0.292732000	-0.132593000
6	-1.624555000	0.374102000	0.694412000
6	-3.007350000	0.270727000	0.363262000
1	-0.440402000	-1.536201000	-1.857091000
1	-7.238100000	3.107826000	2.631503000
1	-5.622255000	3.973845000	-1.240763000
1	-9.047220000	-0.730993000	-0.789965000
1	-6.620650000	-2.662850000	2.165943000
1	5.609112000	4.035781000	1.023102000
1	7.245797000	2.960682000	-2.787517000
1	9.045945000	-0.677798000	0.854286000
1	6.641776000	-2.776981000	-2.004215000
6	-2.995426000	-1.981237000	-2.849412000
6	-1.813527000	-2.629670000	-3.593497000
6	-3.729572000	-1.041729000	-3.838003000
1	-4.601466000	-0.575872000	-3.375005000
1	-3.059992000	-0.248770000	-4.189907000
1	-4.065178000	-1.612100000	-4.712162000
1	-1.106802000	-1.883376000	-3.972462000
1	-2.194327000	-3.189137000	-4.454392000
1	-1.264613000	-3.334492000	-2.959118000
6	-3.953542000	-3.109604000	-2.395567000
1	-3.449000000	-3.792173000	-1.702313000
1	-4.838988000	-2.705849000	-1.901234000
1	-4.279379000	-3.691834000	-3.265591000
6	2.985021000	-1.827169000	2.945092000
6	3.717097000	-0.835911000	3.883387000
6	3.942994000	-2.979567000	2.556142000
1	3.439966000	-3.698305000	1.899309000
1	4.830412000	-2.603818000	2.043579000
1	4.265449000	-3.514171000	3.457331000
1	4.592411000	-0.398964000	3.399135000
1	4.046585000	-1.357125000	4.789953000
1	3.047748000	-0.022818000	4.186326000
6	1.799452000	-2.432379000	3.719172000
1	1.093892000	-1.665339000	4.056791000
1	1.249699000	-3.167589000	3.121025000
1	2.176281000	-2.947243000	4.609127000
6	-1.244293000	1.215932000	1.882203000
1	-1.593155000	0.758370000	2.815936000
1	-0.164718000	1.358990000	1.947738000

1	-1.728951000	2.196243000	1.822495000
6	1.252519000	1.107590000	-1.960325000
1	0.172826000	1.242951000	-2.038652000
1	1.733464000	2.091509000	-1.950738000
1	1.607860000	0.601771000	-2.866275000

29 (R=H; R₁=CH₃, R₂=*tert*-C₄H₉; X=none)

E= -4985.79802 a.u., E_{ZPE}= -4985.13932 a.u.

27	5.841177000	-0.283915000	-0.462652000
8	4.597341000	1.048072000	0.604794000
8	3.904957000	-0.930475000	-0.907099000
8	5.845137000	1.104622000	-1.953361000
8	6.755185000	-1.575146000	-1.720152000
8	7.560761000	0.458417000	0.304335000
8	5.822330000	-1.650759000	1.050469000
6	2.966207000	-0.304194000	-0.371631000
6	1.578357000	-0.638764000	-0.570798000
6	0.652841000	0.141367000	0.084622000
6	1.061687000	1.268487000	0.920576000
6	2.346980000	1.641553000	1.185069000
6	3.370959000	0.851043000	0.517977000
6	6.495482000	1.031524000	-3.035845000
6	7.221413000	-0.068819000	-3.511117000
6	7.283728000	-1.294102000	-2.834642000
6	8.288893000	-0.076449000	1.189728000
6	7.992280000	-1.218758000	1.944787000
6	6.778590000	-1.910481000	1.836732000
1	7.723835000	0.018661000	-4.468362000
1	8.717677000	-1.558159000	2.676193000
1	0.249140000	1.814230000	1.385743000
1	6.625155000	-2.763293000	2.517987000
1	9.249301000	0.425153000	1.391065000
1	6.468620000	1.928263000	-3.676215000
1	7.837891000	-2.111356000	-3.323975000
27	-5.769787000	0.387707000	-0.390924000
8	-5.779695000	1.136990000	1.366136000
8	-7.428062000	-0.524108000	-0.227934000
8	-6.688726000	1.944881000	-0.965929000
8	-5.604053000	-0.401840000	-2.121279000
6	-6.731901000	0.970302000	2.184517000
6	-7.896099000	0.220879000	1.994787000
6	-8.153942000	-0.472528000	0.811438000
6	-6.986729000	2.170492000	-2.178300000
6	-6.725307000	1.359853000	-3.283778000
6	-6.058065000	0.137143000	-3.173964000
1	-8.620732000	0.169976000	2.798418000
1	-7.050209000	1.691188000	-4.262616000
8	-4.058910000	1.196419000	-0.642894000
8	-4.782128000	-1.102886000	0.289825000
6	-3.511141000	-0.895869000	0.247058000
6	-2.525994000	-1.854109000	0.660910000
6	-1.216644000	-1.447494000	0.530628000

6	-0.802206000	-0.154587000	0.052183000
6	-1.737409000	0.787855000	-0.356560000
6	-3.105487000	0.409641000	-0.267744000
1	-0.424095000	-2.120385000	0.834771000
1	-7.510399000	3.120321000	-2.346968000
1	-5.892119000	-0.443121000	-4.091135000
1	-9.084045000	-1.051685000	0.744578000
1	-6.599774000	1.480432000	3.147812000
6	2.732518000	2.801182000	2.110692000
6	1.489364000	3.486109000	2.706852000
6	3.535868000	3.859786000	1.313886000
1	4.459256000	3.443720000	0.907479000
1	2.940334000	4.259120000	0.485240000
1	3.795832000	4.694920000	1.974176000
1	0.847994000	3.921564000	1.932511000
1	1.808905000	4.300922000	3.364227000
1	0.887253000	2.795877000	3.308594000
6	3.596155000	2.261982000	3.278220000
1	3.042948000	1.518226000	3.862825000
1	4.518536000	1.804024000	2.916771000
1	3.863401000	3.086511000	3.948865000
6	-2.936308000	-3.228992000	1.207961000
6	-3.804273000	-3.043829000	2.477097000
6	-1.710579000	-4.079726000	1.587689000
1	-1.064088000	-4.277315000	0.725552000
1	-1.108356000	-3.607481000	2.371785000
1	-2.049471000	-5.047123000	1.971970000
1	-3.245873000	-2.511294000	3.255333000
1	-4.089144000	-4.023668000	2.877593000
1	-4.716078000	-2.484395000	2.260118000
6	-3.743078000	-3.996847000	0.131615000
1	-4.646582000	-3.455298000	-0.154325000
1	-3.137492000	-4.158189000	-0.767255000
1	-4.036751000	-4.978674000	0.520620000
6	1.269122000	-1.783429000	-1.495154000
1	1.531305000	-2.744825000	-1.036829000
1	0.214254000	-1.807643000	-1.772542000
1	1.877228000	-1.703352000	-2.401687000
6	-1.416923000	2.142672000	-0.929269000
1	-2.009216000	2.315345000	-1.833517000
1	-1.685802000	2.944515000	-0.230578000
1	-0.359431000	2.241054000	-1.180301000

30 (R=H, R₁=CH₃, R₂=*tert*-C₄H₉, X=none)

E= -4985.77479 a.u., E_{ZPE}= -4985.12105 a.u.

27	5.903913000	0.326968000	0.461740000
8	4.684117000	-1.105510000	-0.471164000
8	3.959104000	1.053496000	0.749987000
8	5.811756000	-0.857521000	2.112393000
8	6.786380000	1.745201000	1.590932000
8	7.629559000	-0.525690000	-0.140993000
8	5.971905000	1.504208000	-1.196325000

6	3.033999000	0.356930000	0.284499000
6	1.638620000	0.710270000	0.417199000
6	0.731628000	-0.143431000	-0.161472000
6	1.153776000	-1.356949000	-0.853371000
6	2.444757000	-1.766925000	-1.026558000
6	3.454448000	-0.899556000	-0.440643000
6	6.404301000	-0.658713000	3.213061000
6	7.127111000	0.481980000	3.584937000
6	7.251416000	1.606939000	2.759759000
6	8.407868000	-0.108872000	-1.047999000
6	8.167464000	0.942203000	-1.941639000
6	6.963688000	1.658557000	-1.966854000
1	7.576344000	0.511311000	4.571512000
1	8.929278000	1.183455000	-2.674729000
1	0.351165000	-1.955491000	-1.268840000
1	6.852297000	2.427802000	-2.747745000
1	9.364410000	-0.646424000	-1.144832000
1	6.322672000	-1.467396000	3.956787000
1	7.797443000	2.473442000	3.165122000
27	-5.903918000	-0.326981000	0.461718000
8	-4.684112000	1.105526000	-0.471125000
8	-3.959116000	-1.053556000	0.749901000
8	-5.811705000	0.857411000	2.112439000
8	-6.786392000	-1.745262000	1.590846000
8	-7.629560000	0.525744000	-0.140933000
8	-5.971965000	-1.504129000	-1.196409000
6	-3.034005000	-0.356967000	0.284459000
6	-1.638628000	-0.710318000	0.417150000
6	-0.731629000	0.143410000	-0.161471000
6	-1.153769000	1.356964000	-0.853312000
6	-2.444747000	1.766955000	-1.026483000
6	-3.454445000	0.899562000	-0.440615000
6	-6.404227000	0.658548000	3.213108000
6	-7.127050000	-0.482153000	3.584934000
6	-7.251397000	-1.607061000	2.759692000
6	-8.407899000	0.108984000	-1.047939000
6	-8.167535000	-0.942051000	-1.941638000
6	-6.963771000	-1.658423000	-1.966920000
1	-7.576260000	-0.511534000	4.571518000
1	-8.929372000	-1.183255000	-2.674720000
1	-0.351153000	1.955523000	-1.268746000
1	-6.852412000	-2.427630000	-2.747854000
1	-9.364434000	0.646557000	-1.144722000
1	-6.322566000	1.467185000	3.956881000
1	-7.797431000	-2.473577000	3.165016000
6	2.846614000	-3.048084000	-1.765712000
6	1.616915000	-3.798488000	-2.308805000
6	3.598154000	-3.988910000	-0.790179000
1	4.507770000	-3.526105000	-0.403575000
1	2.959595000	-4.262659000	0.057242000
1	3.876778000	-4.910843000	-1.312744000
1	0.936627000	-4.111166000	-1.508637000

1	1.948894000	-4.703988000	-2.826135000
1	1.051548000	-3.197515000	-3.030085000
6	3.765477000	-2.693232000	-2.961042000
1	3.252124000	-2.029372000	-3.665713000
1	4.684788000	-2.206823000	-2.630645000
1	4.036950000	-3.608607000	-3.498309000
6	-2.846595000	3.048151000	-1.765577000
6	-3.598126000	3.988938000	-0.789999000
6	-3.765464000	2.693360000	-2.960921000
1	-3.252117000	2.029529000	-3.665623000
1	-4.684777000	2.206943000	-2.630544000
1	-4.036931000	3.608761000	-3.498146000
1	-4.507741000	3.526120000	-0.403410000
1	-3.876748000	4.910895000	-1.312522000
1	-2.959560000	4.262647000	0.057430000
6	-1.616892000	3.798570000	-2.308639000
1	-0.936600000	4.111208000	-1.508459000
1	-1.051531000	3.197625000	-3.029947000
1	-1.948866000	4.704096000	-2.825928000
6	1.310572000	1.953930000	1.193827000
1	1.645400000	2.850826000	0.659018000
1	0.241792000	2.042490000	1.394238000
1	1.849463000	1.950910000	2.146931000
6	-1.310590000	-1.954019000	1.193718000
1	-0.241809000	-2.042601000	1.394116000
1	-1.849472000	-1.951035000	2.146827000
1	-1.645434000	-2.850885000	0.658871000

31 (R=CF₃; R₁=CH₃, R₂=*tert*-C₄H₉, X=none)

E= -7681.75100 a.u., E_{ZPE}= -7681.05403 a.u.

27	5.573274000	0.203223000	0.045585000
8	5.273522000	1.224319000	1.624693000
8	6.371808000	1.639553000	-0.923768000
8	7.294776000	-0.244085000	0.738296000
8	5.754892000	-0.858009000	-1.524834000
6	5.569051000	2.445383000	1.739397000
6	6.170255000	3.284181000	0.798970000
6	6.525831000	2.803681000	-0.462644000
6	8.124718000	-0.985024000	0.142948000
6	7.977154000	-1.629605000	-1.086652000
6	6.792702000	-1.512576000	-1.816656000
1	6.364801000	4.315285000	1.051794000
1	8.785388000	-2.230387000	-1.474735000
6	5.175499000	3.019834000	3.118446000
9	5.511182000	4.319279000	3.243770000
9	3.843192000	2.920238000	3.294898000
9	5.780648000	2.338340000	4.104734000
6	7.199713000	3.757407000	-1.473490000
9	7.374005000	4.995122000	-0.968884000
9	8.408212000	3.280613000	-1.824657000
9	6.451587000	3.865808000	-2.585116000
6	9.441057000	-1.157807000	0.932356000

9	10.007522000	0.040421000	1.162088000
9	9.199289000	-1.742844000	2.119160000
9	10.335506000	-1.918891000	0.270452000
6	6.655555000	-2.271126000	-3.155616000
9	6.333604000	-1.425755000	-4.147229000
9	7.794674000	-2.903743000	-3.501255000
9	5.682066000	-3.198934000	-3.061494000
8	4.754109000	-1.267482000	0.902239000
8	3.836598000	0.665124000	-0.529589000
6	2.956444000	-0.185144000	-0.096932000
6	1.572681000	-0.052418000	-0.402375000
6	0.735371000	-1.023281000	0.124377000
6	1.258013000	-2.105476000	0.914475000
6	2.588151000	-2.274472000	1.239518000
6	3.469446000	-1.278299000	0.712659000
1	0.531731000	-2.818846000	1.286484000
27	-5.573281000	0.203230000	-0.045525000
8	-5.755111000	-0.858002000	1.524869000
8	-7.294726000	-0.244004000	-0.738422000
8	-6.371853000	1.639589000	0.923754000
8	-5.273323000	1.224323000	-1.624597000
6	-6.792969000	-1.512550000	1.816564000
6	-7.977342000	-1.629540000	1.086425000
6	-8.124754000	-0.984932000	-0.143178000
6	-6.525790000	2.803723000	0.462616000
6	-6.170062000	3.284216000	-0.798958000
6	-5.568791000	2.445400000	-1.739325000
1	-8.785633000	-2.230311000	1.474408000
1	-6.364540000	4.315329000	-1.051797000
6	-6.655990000	-2.271116000	3.155532000
9	-7.795157000	-2.903729000	3.501025000
9	-5.682497000	-3.198932000	3.061518000
9	-6.334154000	-1.425760000	4.147193000
6	-9.441011000	-1.157666000	-0.932735000
9	-10.335552000	-1.918740000	-0.270943000
9	-10.007420000	0.040581000	-1.162507000
9	-9.199127000	-1.742688000	-2.119522000
6	-7.199777000	3.757461000	1.473381000
9	-8.408402000	3.280770000	1.824264000
9	-6.451878000	3.865719000	2.585172000
9	-7.373835000	4.995225000	0.968812000
6	-5.175059000	3.019846000	-3.118325000
9	-5.780096000	2.338365000	-4.104690000
9	-5.510702000	4.319296000	-3.243687000
9	-3.842730000	2.920226000	-3.294610000
8	-3.836641000	0.665057000	0.529820000
8	-4.754094000	-1.267500000	-0.902113000
6	-3.469437000	-1.278320000	-0.712487000
6	-2.588124000	-2.274480000	-1.239337000
6	-1.257995000	-2.105477000	-0.914260000
6	-0.735380000	-1.023293000	-0.124126000
6	-1.572712000	-0.052454000	0.402633000

6	-2.956467000	-0.185186000	0.097153000
1	-0.531695000	-2.818824000	-1.286277000
6	3.113053000	-3.427830000	2.106611000
6	1.976777000	-4.368101000	2.548613000
6	3.788233000	-2.854303000	3.376540000
1	4.630122000	-2.205539000	3.127458000
1	3.071972000	-2.277578000	3.971992000
1	4.160444000	-3.675182000	3.999773000
1	1.226084000	-3.850856000	3.156122000
1	2.395587000	-5.172823000	3.161210000
1	1.472074000	-4.834387000	1.695147000
6	4.139305000	-4.260431000	1.299383000
1	3.683057000	-4.672451000	0.392436000
1	5.003463000	-3.659835000	1.009617000
1	4.495245000	-5.098518000	1.908923000
6	-3.113003000	-3.427823000	-2.106466000
6	-3.788123000	-2.854277000	-3.376416000
6	-4.139305000	-4.260405000	-1.299282000
1	-3.683103000	-4.672434000	-0.392316000
1	-5.003462000	-3.659790000	-1.009552000
1	-4.495238000	-5.098484000	-1.908837000
1	-4.630007000	-2.205495000	-3.127365000
1	-4.160328000	-3.675144000	-3.999668000
1	-3.071827000	-2.277565000	-3.971840000
6	-1.976730000	-4.368114000	-2.548432000
1	-1.225982000	-3.850869000	-3.155872000
1	-1.472097000	-4.834453000	-1.694953000
1	-2.395528000	-5.172799000	-3.161085000
6	-1.144046000	1.091741000	1.278669000
1	-1.221560000	2.046798000	0.744839000
1	-1.801577000	1.169069000	2.150114000
1	-0.114988000	0.973007000	1.620649000
6	1.143984000	1.091791000	-1.278377000
1	1.801516000	1.169168000	-2.149816000
1	0.114931000	0.973036000	-1.620366000
1	1.221463000	2.046833000	-0.744516000

32 (R=CF₃; R₁=CH₃, R₂=*tert*-C₄H₉; X=none)

E= -7681.74568 a.u., E_{ZPE}= -7681.05252 a.u.

27	5.801092000	0.140720000	-0.011232000
8	4.434756000	-0.547682000	1.480233000
8	3.886492000	0.444837000	-0.853636000
8	5.789598000	1.944290000	0.946652000
8	6.849518000	1.026391000	-1.511028000
8	7.487905000	-0.462596000	0.963985000
8	5.784687000	-1.692737000	-0.919884000
6	2.910687000	0.076368000	-0.184916000
6	1.544972000	0.185322000	-0.648272000
6	0.574300000	-0.273130000	0.206304000
6	0.901504000	-0.815171000	1.533606000
6	2.148023000	-0.974302000	2.054419000
6	3.233862000	-0.514928000	1.193188000

6	6.498532000	2.941972000	0.656587000
6	7.327810000	3.118813000	-0.457557000
6	7.415340000	2.148132000	-1.464736000
6	8.196487000	-1.464797000	0.695366000
6	7.922483000	-2.496519000	-0.213851000
6	6.719115000	-2.535279000	-0.927135000
1	7.878232000	4.041369000	-0.565099000
1	8.633601000	-3.300407000	-0.331384000
1	0.046748000	-1.139429000	2.115594000
6	6.360819000	4.106611000	1.664121000
9	5.104069000	4.608522000	1.621396000
9	6.588412000	3.683252000	2.920497000
9	7.210770000	5.125064000	1.413853000
6	8.278049000	2.454168000	-2.711380000
9	8.916233000	3.642415000	-2.630542000
9	9.213823000	1.500622000	-2.882667000
9	7.507934000	2.481906000	-3.818797000
6	6.428709000	-3.762104000	-1.821849000
9	6.187440000	-3.381756000	-3.090569000
9	7.442481000	-4.652928000	-1.846701000
9	5.329819000	-4.412372000	-1.373137000
6	9.497715000	-1.542663000	1.528259000
9	10.191911000	-0.394406000	1.432575000
9	9.204345000	-1.742115000	2.831542000
9	10.312020000	-2.547682000	1.137558000
27	-5.828358000	0.156314000	-0.026948000
8	-5.669771000	1.673964000	-1.162901000
8	-6.845926000	1.056009000	1.306534000
8	-7.444442000	-0.272207000	-0.938380000
8	-5.863885000	-1.382304000	1.092268000
6	-6.171337000	2.802580000	-0.902914000
6	-6.912202000	3.183165000	0.217298000
6	-7.185681000	2.269957000	1.236541000
6	-8.157932000	-1.280600000	-0.677540000
6	-7.930922000	-2.271577000	0.278992000
6	-6.791573000	-2.237967000	1.084713000
1	-7.275788000	4.196317000	0.296761000
1	-8.640607000	-3.076992000	0.391815000
6	-5.876599000	3.846505000	-2.003169000
9	-6.421441000	5.046121000	-1.723565000
9	-4.546327000	4.016760000	-2.132002000
9	-6.363534000	3.433586000	-3.184370000
6	-7.999320000	2.729800000	2.466493000
9	-8.381665000	4.017822000	2.369309000
9	-9.106181000	1.977271000	2.598941000
9	-7.264423000	2.598656000	3.584704000
6	-9.411562000	-1.369552000	-1.575871000
9	-10.122860000	-0.232129000	-1.499339000
9	-9.047712000	-1.554309000	-2.858069000
9	-10.217794000	-2.389502000	-1.222419000
6	-6.565395000	-3.360768000	2.121627000
9	-6.543576000	-2.849893000	3.364296000

9	-7.530233000	-4.299296000	2.073891000
9	-5.385479000	-3.969255000	1.896471000
8	-4.774257000	-0.809967000	-1.269547000
8	-4.185966000	0.633585000	0.779632000
6	-3.183113000	0.097314000	0.158969000
6	-1.843395000	0.289062000	0.591020000
6	-0.859765000	-0.321809000	-0.175960000
6	-1.197575000	-1.087310000	-1.348730000
6	-2.479207000	-1.318026000	-1.796301000
6	-3.511999000	-0.708016000	-1.011638000
1	-0.368657000	-1.531551000	-1.885834000
6	2.440728000	-1.578036000	3.431596000
6	3.160542000	-0.526072000	4.313280000
6	3.340145000	-2.829007000	3.266993000
1	2.852515000	-3.584473000	2.640990000
1	4.305036000	-2.578569000	2.823042000
1	3.524983000	-3.275579000	4.249855000
1	4.116362000	-0.220278000	3.884398000
1	3.353527000	-0.952738000	5.303404000
1	2.538039000	0.365420000	4.447786000
6	1.144999000	-2.004634000	4.144203000
1	0.474330000	-1.157007000	4.324407000
1	0.597509000	-2.770675000	3.583471000
1	1.397760000	-2.432269000	5.119026000
6	-2.806366000	-2.156139000	-3.039675000
6	-3.695840000	-3.358910000	-2.640002000
6	-1.530234000	-2.703875000	-3.704874000
1	-0.864186000	-1.902584000	-4.043666000
1	-0.967161000	-3.366046000	-3.037660000
1	-1.808292000	-3.288987000	-4.586727000
1	-3.186733000	-3.998023000	-1.910217000
1	-3.912345000	-3.965617000	-3.525902000
1	-4.645708000	-3.032167000	-2.212722000
6	-3.550996000	-1.274961000	-4.073696000
1	-4.492530000	-0.891335000	-3.676272000
1	-2.932579000	-0.424199000	-4.380403000
1	-3.773913000	-1.867361000	-4.967880000
6	1.322957000	0.811029000	-1.996041000
1	0.274153000	1.060335000	-2.161828000
1	1.924227000	1.721075000	-2.085921000
1	1.656333000	0.144477000	-2.800551000
6	-1.603821000	1.165086000	1.790759000
1	-2.164525000	2.100019000	1.690327000
1	-1.965489000	0.688067000	2.709547000
1	-0.548282000	1.411045000	1.916016000

33 (R=CF₃; R₁=CH₃, R₂=*tert*-C₄H₉; X=none)

E= -7681.73498 a.u., E_{ZPE}= -7681.04576 a.u.

27	5.922156000	0.111304000	0.021430000
8	4.608104000	-0.910000000	1.345979000
8	3.988439000	0.402397000	-0.803068000
8	5.709726000	1.711247000	1.267992000

8	6.884984000	1.352019000	-1.263785000
8	7.638845000	-0.503390000	0.914010000
8	6.093921000	-1.499117000	-1.215541000
6	3.039079000	-0.092327000	-0.184393000
6	1.658885000	0.034818000	-0.615548000
6	0.724424000	-0.570181000	0.179188000
6	1.082765000	-1.290673000	1.407227000
6	2.342062000	-1.475329000	1.890252000
6	3.400645000	-0.868020000	1.087871000
6	6.305009000	2.817173000	1.177789000
6	7.123843000	3.272074000	0.138542000
6	7.328393000	2.501981000	-1.014672000
6	8.462991000	-1.339163000	0.462275000
6	8.313852000	-2.179305000	-0.649378000
6	7.121302000	-2.207547000	-1.381037000
1	7.569760000	4.253149000	0.205627000
1	9.115194000	-2.852112000	-0.915834000
1	0.246589000	-1.716440000	1.950394000
6	6.030142000	3.758341000	2.372618000
9	4.706255000	4.022785000	2.458212000
9	6.407358000	3.180561000	3.528325000
9	6.673847000	4.939504000	2.273767000
6	8.159502000	3.106432000	-2.170534000
9	8.731520000	4.284800000	-1.842917000
9	9.141046000	2.262992000	-2.537887000
9	7.372050000	3.320831000	-3.245702000
6	6.971163000	-3.251874000	-2.510731000
9	6.587560000	-2.664289000	-3.658091000
9	8.110791000	-3.930273000	-2.756230000
9	6.022573000	-4.158408000	-2.176307000
6	9.762177000	-1.437656000	1.295454000
9	10.331810000	-0.225882000	1.427517000
9	9.486967000	-1.904269000	2.531634000
9	10.676492000	-2.263251000	0.742474000
27	-5.922155000	0.111301000	-0.021404000
8	-4.608114000	-0.910020000	-1.345952000
8	-3.988431000	0.402378000	0.803090000
8	-5.709703000	1.711223000	-1.267998000
8	-6.884946000	1.352054000	1.263797000
8	-7.638859000	-0.503353000	-0.913989000
8	-6.093953000	-1.499116000	1.215561000
6	-3.039073000	-0.092322000	0.184392000
6	-1.658874000	0.034813000	0.615537000
6	-0.724421000	-0.570170000	-0.179219000
6	-1.082776000	-1.290664000	-1.407255000
6	-2.342078000	-1.475304000	-1.890273000
6	-3.400651000	-0.868012000	-1.087870000
6	-6.304962000	2.817161000	-1.177804000
6	-7.123786000	3.272091000	-0.138559000
6	-7.328341000	2.502018000	1.014667000
6	-8.463016000	-1.339119000	-0.462262000
6	-8.313890000	-2.179274000	0.649383000

6	-7.121344000	-2.207534000	1.381049000
1	-7.569687000	4.253172000	-0.205657000
1	-9.115238000	-2.852078000	0.915827000
1	-0.246608000	-1.716459000	-1.950410000
6	-6.030077000	3.758314000	-2.372641000
9	-4.706188000	4.022747000	-2.458225000
9	-6.407285000	3.180523000	-3.528346000
9	-6.673774000	4.939483000	-2.273811000
6	-8.159447000	3.106493000	2.170519000
9	-8.731473000	4.284851000	1.842878000
9	-9.140983000	2.263057000	2.537899000
9	-7.371989000	3.320922000	3.245677000
6	-6.971216000	-3.251877000	2.510729000
9	-6.587633000	-2.664306000	3.658103000
9	-8.110843000	-3.930286000	2.756202000
9	-6.022615000	-4.158401000	2.176306000
6	-9.762194000	-1.437604000	-1.295455000
9	-10.331811000	-0.225826000	-1.427539000
9	-9.486975000	-1.904236000	-2.531627000
9	-10.676524000	-2.263182000	-0.742476000
6	2.671417000	-2.240502000	3.174715000
6	3.379338000	-1.287736000	4.172226000
6	3.599616000	-3.436075000	2.842018000
1	3.121694000	-4.120888000	2.132843000
1	4.551427000	-3.106603000	2.422013000
1	3.810508000	-3.996467000	3.758677000
1	4.320693000	-0.905022000	3.774382000
1	3.597893000	-1.831390000	5.097264000
1	2.737312000	-0.437353000	4.426922000
6	1.397914000	-2.786227000	3.845152000
1	0.707981000	-1.986254000	4.136747000
1	0.861556000	-3.493975000	3.202800000
1	1.675604000	-3.321576000	4.757707000
6	-2.671472000	-2.240513000	-3.174705000
6	-1.398009000	-2.786326000	-3.845149000
6	-3.379378000	-1.287766000	-4.172245000
1	-4.320682000	-0.904952000	-3.774374000
1	-2.737303000	-0.437448000	-4.427036000
1	-3.598025000	-1.831468000	-5.097232000
1	-0.708154000	-1.986388000	-4.137022000
1	-1.675769000	-3.321912000	-4.757543000
1	-0.861540000	-3.493886000	-3.202682000
6	-3.599718000	-3.436025000	-2.841931000
1	-3.121815000	-4.120822000	-2.132728000
1	-4.551506000	-3.106484000	-2.421924000
1	-3.810654000	-3.996455000	-3.758556000
6	1.391422000	0.831776000	-1.858991000
1	0.324641000	0.978171000	-2.033484000
1	1.869601000	1.814203000	-1.784054000
1	1.832439000	0.345063000	-2.736631000
6	-1.391393000	0.831724000	1.859005000
1	-1.832384000	0.344972000	2.736636000

1	-0.324609000	0.978121000	2.033480000
1	-1.869585000	1.814149000	1.784117000