Appendix A

Molecular Coordinates

Appendix A

Molecular Coordinates

Ethylene, 6-311++G Basis (Nuclear Rep. = 33.663966)**

Z-matrix Coordinates (Å and °)

Atom	Center A	Distance	Center B	Angle	Center C	Dihedral
C						
C	1	RCC				
H	2	RCH	1	ANG1		
H	2	RCH	1	ANG1	3	180.0
H	1	RCH	2	ANG1	3	0.0
H	1	RCH	2	ANG1	3	180.0

Variable	Value
RCC	1.3185
RCH	1.0766
ANG1	121.6612

Cartesian Coordinates in Å

Atom	At. No.	X	Y	Z
C	6	0.0	0.0	0.659250
C	6	0.0	0.0	-0.659250
H	1	0.0	0.916366	-1.224352
H	1	0.0	-0.916366	-1.224352
H	1	0.0	0.916366	1.224352
H	1	0.0	-0.916366	1.224352

Ethylene, cc-pVTZ Basis (Nuclear Rep. = 33.756981)

Z-matrix Coordinates (Å and °)

Atom	Center A	Distance	Center B	Angle	Center C	Dihedral
C						
C	1	RCC				
H	2	RCH	1	ANG1		
H	2	RCH	1	ANG1	3	180.0
H	1	RCH	2	ANG1	3	0.0
H	1	RCH	2	ANG1	3	180.0

Variable	Value
RCC	1.3144
RCH	1.0741
ANG1	121.6537

Cartesian Coordinates in Å

Atom	At. No.	X	Y	Z
C	6	0.0	0.0	0.657200
C	6	0.0	0.0	-0.657200
H	1	0.0	0.914312	-1.220870
H	1	0.0	-0.914312	-1.220870
H	1	0.0	0.914312	1.220870
H	1	0.0	-0.914312	1.220870

Ethylene, 6-311++G(3df,3pd) Basis (Nuclear Rep. = 33.756981)

Z-matrix Coordinates (Å and °)

Atom	Center A	Distance	Center B	Angle	Center C	Dihedral
C						
C	1	RCC				
H	2	RCH	1	ANG1		
H	2	RCH	1	ANG1	3	180.0
H	1	RCH	2	ANG1	3	0.0
H	1	RCH	2	ANG1	3	180.0

Variable	Value
RCC	1.3144
RCH	1.0741
ANG1	121.6537

Cartesian Coordinates in Å

Atom	At. No.	X	Y	Z
C	6	0.0	0.0	0.657200
C	6	0.0	0.0	-0.657200
H	1	0.0	0.914312	-1.220870
H	1	0.0	-0.914312	-1.220870
H	1	0.0	0.914312	1.220870
H	1	0.0	-0.914312	1.220870

Isobutene, 6-311++G and cc-pVTZ Basis Sets (Nuclear Rep. = 120.116981)**

Z-matrix Coordinates (Å and °)

Atom	Center A	Distance	Center B	Angle	Center C	Dihedral
C						
C	1	RCC1				
C	1	RCC2	2	CCC		
C	1	RCC2	2	CCC	3	180.0
H	2	RCH1	1	CCH1	3	0.0
H	2	RCH1	1	CCH1	4	0.0
H	3	RCH2	1	CCH2	2	-DIHE3
H	3	RCH2	1	CCH2	2	DIHE3
H	3	RCH3	1	CCH3	2	0.0
H	4	RCH2	1	CCH2	2	DIHE3
H	4	RCH2	1	CCH2	2	-DIHE3
H	4	RCH3	1	CCH3	2	0.0

Variable	Value
RCC1	1.3224
RCC2	1.5073
CCC	122.2419
RCH1	1.0766
CCH1	121.6245
RCH2	1.0878
CCH2	110.5765
DIHE3	120.8021
RCH3	1.0836
CCH3	111.7128

Cartesian Coordinates in Å

Atom	At. No.	X	Y	Z
C	6	0.0	0.0	0.127225
C	6	0.0	0.0	1.449625
C	6	0.0	1.274879	-0.676912
C	6	0.0	-1.274879	-0.676912
H	1	0.0	0.916728	2.014140
H	1	0.0	-0.916728	2.014140
H	1	-0.874748	1.320027	-1.321960
H	1	0.874748	1.320027	-1.321960
H	1	0.0	2.151026	-0.039295
H	1	-0.874748	-1.320027	-1.321960
H	1	0.874748	-1.320027	-1.321960
H	1	0.0	-2.151026	-0.039295

Imidazole, 6-311++G Basis Set (Nuclear Rep. = 164.969257)**

Z-matrix Coordinates (Å and °)

Atom	Center A	Distance	Center B	Angle	Center C	Dihedral
N						
C	1	RN1C1				
N	2	RC1N2	1	ANG1		
C	3	RN2C2	2	ANG2	1	0.0
C	4	RC2C3	3	ANG3	2	0.0
H	2	RC1H1	1	ANG4	5	180.0
H	3	RN2H2	2	ANG5	6	0.0
H	4	RC2H3	3	ANG6	7	0.0
H	5	RC3H4	4	ANG7	8	0.0

Variable	Value
RN1C1	1.2878
RC1N2	1.3499
ANG1	112.128
RN2C2	1.3725
ANG2	106.7994
RC2C3	1.3507
ANG3	105.2405
RC1H1	1.0713
ANG4	125.5984
RN2H2	0.9919
ANG5	126.3916
RC2H3	1.0684
ANG6	122.5807
RC3H4	1.0697
ANG7	128.0903

Cartesian Coordinates in Å

Atom	At. No.	X	Y	Z
N	7	-0.741162	-0.964252	0.0
C	6	-1.075551	0.279377	0.0
N	7	0.0	1.095109	0.0
C	6	1.110055	0.287933	0.0
C	6	0.630803	-0.974885	0.0
H	1	-2.078690	0.655404	0.0
H	1	-0.013611	2.086916	0.0
H	1	2.104819	0.677707	0.0
H	1	1.183777	-1.890569	0.0

Imidazole, cc-pVTZ Basis Set (Nuclear Rep. = 165.316445)

Z-matrix Coordinates (Å and °)

Atom	Center A	Distance	Center B	Angle	Center C	Dihedral
N						
C	1	RN1C1				
N	2	RC1N2	1	ANG1		
C	3	RN2C2	2	ANG2	1	0.0
C	4	RC2C3	3	ANG3	2	0.0
H	2	RC1H1	1	ANG4	5	180.0
H	3	RN2H2	2	ANG5	6	0.0
H	4	RC2H3	3	ANG6	7	0.0
H	5	RC3H4	4	ANG7	8	0.0

Variable	Value
RN1C1	1.2860
RC1N2	1.3458
ANG1	112.184
RN2C2	1.3693
ANG2	106.817
RC2C3	1.3474
ANG3	105.271
RC1H1	1.0695
ANG4	125.569
RN2H2	0.9890
ANG5	126.377
RC2H3	1.0664
ANG6	122.600
RC3H4	1.0678
ANG7	128.065

Cartesian Coordinates in Å

Atom	At. No.	X	Y	Z
N	7	-0.740438	-0.962630	0.0
C	6	-1.072627	0.279725	0.0
N	7	0.0	1.092529	0.0
C	6	1.107368	0.287099	0.0
C	6	0.629795	-0.972826	0.0
H	1	-2.073751	0.655999	0.0
H	1	-0.013412	2.081438	0.0
H	1	2.100446	0.675694	0.0
H	1	1.182562	-1.886415	0.0

Caffeine, 3-21G and 6-31G Basis Sets (Nuclear Rep. = 916.319741)**

Z-matrix Coordinates (Å and °)

Atom	Center A	Distance	Center B	Angle	Center C	Dihedral
N						
C	1	RN1C1				
N	2	RC1N2	1	ANG1		
C	3	RN2C2	2	ANG2	1	0.
C	4	RC2C3	3	ANG3	2	0.
C	3	RN3C6	2	ANG5	1	180.
H	6	RC6H7	3	ANG6	2	DIHE1
H	6	RC6H8	3	ANG7	2	DIHE2
H	6	RC6H9	3	ANG8	2	DIHE3
C	4	RC4C10	5	ANG9	2	180.
O	10	RC10O11	4	ANG10	3	0.
N	10	RC10N12	4	ANG11	3	180.
C	12	RN12C13	10	ANG12	4	180.
H	13	RC13H14	12	ANG13	10	DIHE4
H	13	RC13H15	12	ANG14	10	DIHE5
H	13	RC13H16	12	ANG15	10	DIHE6
C	12	RN12C17	10	ANG16	4	0.
O	17	RC17O18	12	ANG17	10	180.
N	17	RC17N19	12	ANG18	10	0.
C	19	RN19C20	17	ANG19	12	180.
H	20	RC20H21	19	ANG20	10	DIHE11
H	20	RC20H22	19	ANG21	10	DIHE12
H	20	RC20H23	19	ANG22	10	DIHE13

Variable	Value
RN1C1	1.3087
RC1N2	1.3489
ANG1	114.5714
RN2C2	1.3945
ANG2	104.4811
RC2C3	1.3626
ANG3	106.2146
RN3C6	1.47
ANG5	128.9068
RC6H7	1.0807
ANG6	109.9109
DIHE1	299.5553
RC6H8	1.0807
ANG7	109.904
DIHE2	60.552
RC6H9	1.0765
ANG8	107.0593
DIHE3	180.044
RC4C10	1.424
ANG9	122.4338
RC10O11	1.2228
ANG10	126.254
RC10N12	1.3956
ANG11	111.7592
RN12C13	1.4778
ANG12	118.0931

Variable	Value
RC13H14	1.0746
ANG13	107.4187
DIHE4	360.1356
RC13H15	1.0792
ANG14	109.572
DIHE5	120.4648
RC13H16	1.0793
ANG15	109.5885
DIHE6	239.811
RN12C17	1.3935
ANG16	126.8636
RC17O18	1.2147
ANG17	121.2827
RC17N19	1.3766
ANG18	117.0862
RN19C20	1.4719
ANG19	118.5543
RC20H21	1.0797
ANG20	109.7104
DIHE11	300.1115
RC20H22	1.0797
ANG21	109.7318
DIHE12	59.782
RC20H23	1.0768
ANG22	107.5607
DIHE13	179.9684

Cartesian Coordinates in Å

Atom	At. No.	X	Y	Z
N	7	1.228476	-2.127881	-0.000008
C	6	2.386568	-1.518357	-0.000001
N	7	2.311572	-0.171544	0.000005
C	6	0.944076	0.101558	0.000001
C	6	0.314717	-1.106990	-0.000007
C	6	3.402380	0.813869	0.000013
H	1	4.011462	0.688664	0.883900
H	1	4.010282	0.689803	-0.884845
H	1	2.946841	1.789233	0.000806
C	6	0.230834	1.334060	0.000003
O	8	0.722107	2.453833	0.000010
N	7	-1.150153	1.132633	-0.000003
C	6	-2.026933	2.322234	-0.000001
H	1	-1.392426	3.189506	-0.002421
H	1	-2.656429	2.307381	-0.876464
H	1	-2.653224	2.310145	0.878920
C	6	-1.816465	-0.091242	-0.000011
O	8	-3.029799	-0.148835	-0.000016
N	7	-1.039749	-1.227789	-0.000013
C	6	-1.710197	-2.538129	-0.000022
H	1	-2.330029	-2.630036	0.879247
H	1	-2.331588	-2.629653	-0.878229
H	1	-0.944250	-3.294979	-0.000588

18-crown-6, 3-21G Basis (Nuclear Rep. = 1485.9218009)

	Cartesian Coordinates in Å		
Atom	X	Y	Z
O	-2.852953	-2.134361	-0.141930
O	2.852953	2.134361	0.141930
C	-1.614812	-1.627784	0.360229
C	1.614812	1.627784	-0.360229
C	-0.525733	-2.438177	-0.335927
C	0.525733	2.438177	0.335927
O	0.698049	-2.066187	0.295152
O	-0.698049	2.066187	-0.295152
C	1.828020	-2.675136	-0.324822
C	-1.828020	2.675136	0.324822
C	3.061549	-2.086443	0.352453
C	-3.061549	2.086443	-0.352453
O	3.396054	-0.900601	-0.361791
O	-3.396054	0.900601	0.361791
C	4.101957	0.057978	0.421232
C	-4.101957	-0.057978	-0.421232
C	3.979847	1.395299	-0.304190
C	-3.979847	-1.395299	0.304190
H	-1.515266	-0.533904	0.126301
H	1.515266	0.533904	-0.126301
H	-1.572378	-1.776284	1.470718
H	1.572378	1.776284	-1.470718
H	-0.700807	-3.538236	-0.205824
H	0.700807	3.538236	0.205824
H	-0.489048	-2.195589	-1.429810
H	0.489048	2.195589	1.429810
H	1.790377	-3.784455	-0.161639
H	-1.790377	3.784455	0.161639
H	1.834505	-2.451386	-1.4240991
H	-1.834505	2.451386	1.424099
H	3.922018	-2.801991	0.272858
H	-3.922018	2.801991	-0.272858
H	2.845607	-1.867358	1.430933
H	-2.845607	1.867358	-1.430933
H	3.666580	0.133909	1.452229
H	-3.666580	-0.133909	-1.452229
H	5.177195	-0.255057	0.488254
H	-5.177195	0.255057	-0.488254
H	4.851875	2.050672	-0.036884
H	-4.851875	-2.050672	0.036884
H	3.936261	1.235602	-1.413295
H	-3.936261	-1.235602	1.413295

18-crown-6, 6-31G Basis (Nuclear Rep. = 1493.514706)**

Cartesian Coordinates in Å

Atom	X	Y	Z
O	2.6513	2.1644	-0.2345
O	-2.6513	-2.1644	0.2345
O	-0.8671	2.1450	0.2755
O	0.8671	-2.1450	-0.2755
C	1.4420	1.7551	0.3491
C	-1.4420	-1.7551	-0.3491
C	0.3399	2.5863	-0.2725
C	-0.3399	-2.5863	0.2725
C	-2.0160	2.7318	-0.2485
C	2.0160	-2.7318	0.2485
C	-3.2208	1.9840	0.2751
C	3.2208	-1.9840	-0.2751
O	-3.2382	0.7133	-0.2991
O	3.2382	-0.7133	0.2991
C	-4.1103	-0.2095	0.2800
C	4.1103	0.2095	-0.2800
C	-3.8200	-1.5925	-0.2730
C	3.8200	1.5925	0.2730
H	1.2512	0.7061	0.1728
H	-1.2512	-0.7061	-0.1728
H	1.4636	1.9204	1.4251
H	-1.4636	-1.9204	-1.4251
H	0.5000	3.6443	-0.0673
H	-0.5000	-3.6443	0.0673
H	0.3460	2.4511	-1.3525
H	-0.3460	-2.4511	1.3525
H	-2.0820	3.7799	0.0470
H	2.0820	-3.7799	-0.0470
H	-2.0105	2.6885	-1.3362
H	2.0105	-2.6885	1.3362
H	-4.1302	2.5317	0.0214
H	4.1302	-2.5317	-0.0214
H	-3.1560	1.9170	1.3585
H	3.1560	-1.9170	-1.3585
H	-3.9905	-0.2256	1.3619
H	3.9905	0.2256	-1.3619
H	-5.1464	0.0553	0.0590
H	5.1464	-0.0553	-0.0590
H	-4.6310	-2.2531	0.0169
H	4.6310	2.2531	-0.0169
H	-3.7913	-1.5467	-1.3573
H	3.7913	1.5467	1.3573

s18-crown-6, 6-31G Basis (Nuclear Rep. = 6023.39046)**

Cartesian Coordinates in Å

C	2.20589351	2.56835271	-2.27834431
H	2.64708251	3.55958304	-2.32833119
H	2.52337376	2.12287548	-1.34172135
C	2.68131698	1.71330539	-3.45264140
H	3.75180751	1.54996509	-3.38227741
H	2.51147658	2.24762242	-4.38616034
C	1.95281563	0.36257292	-3.50537956
H	2.21176375	-0.20046505	-2.61268662
C	2.39496956	-0.43928297	-4.73224464
H	3.47759234	-0.48872873	-4.77515365
H	2.02708693	-1.45864874	-4.71283876
H	2.05364872	0.02423976	-5.65410759
O	-1.24263489	3.51219195	1.32837879
C	-1.78937397	4.24810106	0.26011987
H	-1.45171363	5.28181098	0.32437799
H	-2.86071859	4.23693298	0.39609386
C	-1.39846288	3.64248259	-1.08963020
H	-1.86468450	2.66530509	-1.16264031
C	-1.90157038	4.52690507	-2.23217310
H	-1.38815684	5.48413652	-2.25193999
H	-1.76834953	4.05557618	-3.19854315
H	-2.96186931	4.72650134	-2.11690908
C	1.94909650	0.38799281	3.72482145
H	2.23851562	-0.17144452	2.83920938
C	2.37854609	-0.40571287	4.96130436
H	2.04779089	-1.43680627	4.92121124
H	3.46041063	-0.41898725	5.03832436
H	1.99258037	0.03989135	5.87468741
C	2.64751842	1.75625079	3.69347060
H	2.44238587	2.28168732	4.62484366
H	3.72306767	1.61975693	3.64772259
C	2.18280731	2.60936842	2.51231670
H	2.54584144	2.18181375	1.58309565
H	2.59180226	3.61305447	2.58603881
O	0.51052011	2.75942544	0.08299771
C	0.12363395	3.44389543	-1.09737222
H	0.60391845	4.42248052	-1.09433010
C	-0.43326599	-0.62746306	3.65432832
H	-0.14799926	-1.21300599	4.52498326
O	-0.11917894	-1.37296543	2.49150424
C	0.68520093	2.68400982	-2.29432830
H	0.38844917	3.22502484	-3.19031524
C	-0.65923210	-2.67147456	2.47317609
H	-0.29017874	-3.21534621	3.34005603
C	-0.43906942	-0.62503929	-3.47289568
H	-0.18224013	-1.19527183	-4.36286574
C	0.13062009	3.41311278	1.25702478
H	0.56736097	4.41240713	1.25192790
O	0.10055094	1.39873357	-2.33465145
C	-2.18280731	-2.60936842	2.51231670
H	-2.54584144	-2.18181375	1.58309565
H	-2.59180226	-3.61305447	2.58603881
C	-2.64751842	-1.75625079	3.69347060

H	-2.44238587	-2.28168732	4.62484366
H	-3.72306767	-1.61975693	3.64772259
C	-1.94909650	-0.38799281	3.72482145
H	-2.23851562	0.17144452	2.83920938
C	-2.37854609	0.40571287	4.96130436
H	-1.99258037	-0.03989135	5.87468741
H	-2.04779089	1.43680627	4.92121124
H	-3.46041063	0.41898725	5.03832436
C	1.39846288	-3.64248259	-1.08963020
H	1.86468450	-2.66530509	-1.16264031
C	1.90157038	-4.52690507	-2.23217310
H	1.76834953	-4.05557618	-3.19854315
H	2.96186931	-4.72650134	-2.11690908
H	1.38815684	-5.48413652	-2.25193999
C	1.78937397	-4.24810106	0.26011987
H	1.45171363	-5.28181098	0.32437799
H	2.86071859	-4.23693298	0.39609386
O	1.24263489	-3.51219195	1.32837879
C	0.43326599	0.62746306	3.65432832
H	0.14799926	1.21300599	4.52498326
C	-0.12363395	-3.44389543	-1.09737222
H	-0.60391845	-4.42248052	-1.09433010
O	0.11917894	1.37296543	2.49150424
O	-0.51052011	-2.75942544	0.08299771
C	-0.13062009	-3.41311278	1.25702478
H	-0.56736097	-4.41240713	1.25192790
C	0.43906942	0.62503929	-3.47289568
H	0.18224013	1.19527183	-4.36286574
O	-0.10055094	-1.39873357	-2.33465145
C	0.65923210	2.67147456	2.47317609
H	0.29017874	3.21534621	3.34005603
C	-0.68520093	-2.68400982	-2.29432830
H	-0.38844917	-3.22502484	-3.19031524
C	-1.95281563	-0.36257292	-3.50537956
H	-2.21176375	0.20046505	-2.61268662
C	-2.39496956	0.43928297	-4.73224464
H	-3.47759234	0.48872873	-4.77515365
H	-2.02708693	1.45864874	-4.71283876
H	-2.05364872	-0.02423976	-5.65410759
C	-2.68131698	-1.71330539	-3.45264140
H	-2.51147658	-2.24762242	-4.38616034
H	-3.75180751	-1.54996509	-3.38227741
C	-2.20589351	-2.56835271	-2.27834431
H	-2.52337376	-2.12287548	-1.34172135
H	-2.64708251	-3.55958304	-2.32833119