Supporting Information to Chapter 17

Biomimetic Approaches to Reversible CO_2 Capture From Air. *N*-Methylcarbaminic Acid Formation in Rubisco-Inspired Models

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Abstract: We are interested in the design and development of rubisco-based biomimetic systems for reversible CO_2 capture from air. In this chapter, we review the enzyme mechanism of rubisco-based biological CO_2 fixation, we identify the carbamoylation reaction of the activator CO_2 in the active site of rubisco as a promising candidate for the development of a chemical CO_2 capture and release system, we discuss the construction of several small molecule models {CO_2, CH_3NH_2, (aldehyde/ketone), magnesium formate} and describe the equations for their thermochemical assessment, and we present the results of computational studies of small molecule models to assess the thermochemistry of the carbamoylation reaction. The Mg^{2+}-catalyzed formation of carbonyl-aggregates of *N*-methylcarbaminic acid (NMCA) is rather exergonic and it is only for the thermochemistry of the water/CO_2 ligand exchange reaction that the reversal of NMCA formation becomes possible. The thermochemistry of the CO_2 capture reaction is discussed ($\Delta H(T_1) < \Delta G(T_1) < 0$) and the condition for CO_2 release by temperature variations ($\Delta T \cdot |\Delta S(T_1)| > |\Delta G(T_1)|$) emphasizes the need to develop CO_2 capture reactions with negative reaction entropies $\Delta S(T_1)$ of substantial magnitude ($|\Delta S(T_1)| \approx 80$ - 60 cal mol^{-1} K^{-1}).

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Cartesian Coordinates of Stationary Structures
Structures of Small Systems

OCO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000088
2	8	0	0.000000	-1.169131	-0.000033
3	8	0	0.000000	1.169131	-0.000033

H_2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.119749
2	1	0	0.000000	0.761580	-0.478994
3	1	0	0.000000	-0.761580	-0.478994

CH_3NH_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.752364	0.000000	-0.126188
2	1	0	-1.142542	-0.812191	0.348899
3	1	0	-1.142542	0.812191	0.348899
4	6	0	0.705751	0.000000	0.017594
5	1	0	1.115509	-0.881664	-0.487282
6	1	0	1.115509	0.881664	-0.487281
7	1	0	1.086109	0.000000	1.054517

$Mg(O_2CH)_2$ (= MgL_2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.703782	-0.770954	0.796380
2	8	0	-1.705935	0.770105	-0.796133
3	1	0	-3.426644	0.000809	0.003694
4	8	0	1.706387	-0.796749	-0.769311
5	8	0	1.703306	0.798031	0.769555
6	1	0	3.426631	0.000290	0.003839
7	6	0	-2.327827	-0.000051	0.001374
8	6	0	2.327814	0.000354	0.001719
9	12	0	0.000023	-0.000532	-0.002502

H_2CO (= FA)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-0.528958
2	1	0	0.000000	0.937885	-1.123675
3	1	0	0.000000	-0.937885	-1.123675
4	8	0	0.000000	0.000000	0.677637

$(CH_3)_2CO$ (= Ac)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000026	0.185343	0.000000
2	8	0	0.000044	1.401009	0.000000
3	6	0	-0.000026	-0.614820	1.293090
4	1	0	0.881159	-1.267064	1.341454
5	1	0	-0.000273	0.063500	2.148551
6	1	0	-0.880829	-1.267578	1.341293
7	6	0	-0.000026	-0.614820	-1.293090
8	1	0	0.881159	-1.267064	-1.341454
9	1	0	-0.880829	-1.267578	-1.341293
10	1	0	-0.000273	0.063500	-2.148551

$CH_3NH_2{\bullet}OCH_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.120683	-0.292753	0.486898
2	1	0	-0.395586	0.424356	0.495584
3	1	0	-1.447147	-0.380011	1.447856
4	6	0	-2.229474	0.124310	-0.374847
5	1	0	-1.862406	0.240077	-1.400525
6	1	0	-2.994768	-0.659960	-0.389877
7	1	0	-2.722909	1.069579	-0.089082
8	8	0	1.812925	0.686268	0.094545
9	6	0	1.995367	-0.472174	-0.210948
10	1	0	1.170016	-1.207245	-0.204004
11	1	0	2.998821	-0.840483	-0.509828

$CH_3NH_2{\bullet}OC(CH_3)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.247644	0.196809	-0.513116
2	1	0	-1.429573	-0.407137	-0.423519
3	1	0	-2.607998	0.052585	-1.455190
4	6	0	-3.265631	-0.186179	0.467069

5	1	0	-2.859366	-0.052875	1.475881
6	1	0	-4.132272	0.478925	0.375591
7	1	0	-3.631650	-1.225397	0.391577
8	8	0	0.649438	-1.018005	-0.180681
9	6	0	1.439451	-0.103137	-0.012308
10	6	0	2.924230	-0.377682	0.154135
11	1	0	3.492814	0.112741	-0.646158
12	1	0	3.288299	0.038395	1.101745
13	1	0	3.110809	-1.453077	0.128278
14	6	0	0.999578	1.347301	0.042038
15	1	0	1.260820	1.778782	1.017284
16	1	0	1.538776	1.934461	-0.712530
17	1	0	-0.078428	1.427154	-0.121303

$CH_3NH_2 \bullet CO_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.416463	0.156225	0.004940
2	8	0	-1.840665	-0.932955	0.060009
3	8	0	-1.088363	1.278531	-0.047607
4	6	0	2.198644	0.355844	0.071181
5	1	0	2.010617	1.105205	-0.704121
6	1	0	2.034076	0.842802	1.037684
7	1	0	3.259607	0.060902	0.013875
8	7	0	1.236819	-0.740821	-0.081894
9	1	0	1.388989	-1.216513	-0.969677
10	1	0	1.388118	-1.443667	0.639556

$H_2O \bullet CO_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.894689	-0.150951	-0.105586
2	1	0	-2.050580	0.771803	0.145366
3	1	0	-2.327854	-0.666141	0.591299
4	6	0	0.866776	0.045982	0.000925
5	8	0	0.721019	1.207519	0.014442
6	8	0	1.070892	-1.104262	-0.001633

$(HCO_2)_2Mg \bullet CO_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.021572	-0.458747	1.215811
2	8	0	-2.109418	-0.733253	-0.980472
3	1	0	-3.540236	-1.467431	0.284862
4	8	0	1.064217	1.204216	0.856358
5	8	0	-0.083049	2.123916	-0.798495

6	1	0	1.510439	3.049723	0.088659
7	8	0	3.155934	-1.419483	0.153686
8	8	0	0.913670	-1.294567	-0.493603
9	6	0	-2.597789	-0.910578	0.175753
10	6	0	0.858478	2.164264	0.051154
11	6	0	2.042715	-1.335710	-0.153943
12	12	0	-0.595740	0.294432	-0.036465

$(HCO_2)_2Mg{\bullet}OH_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.492622	-0.891539	1.048035
2	8	0	1.894198	0.042306	-0.921913
3	1	0	3.342904	-0.893378	0.178967
4	8	0	-1.861727	0.117491	0.927080
5	8	0	-1.559926	-0.905143	-1.017390
6	1	0	-3.374728	-0.820453	-0.081095
7	6	0	2.285659	-0.593492	0.103009
8	6	0	-2.308465	-0.546158	-0.055602
9	12	0	-0.006917	0.000487	-0.041052
10	8	0	0.019782	2.069667	-0.069137
11	1	0	0.862628	2.525426	-0.218183
12	1	0	-0.490555	2.558203	0.595104

Methylamine Solvated by Water

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.755917	0.738635	0.052278
2	1	0	-0.798083	1.173104	-0.868313
3	1	0	-1.341272	1.305148	0.663357
4	6	0	-1.266319	-0.638712	-0.021542
5	1	0	-0.558905	-1.235630	-0.603745
6	1	0	-1.299848	-1.058858	0.988827
7	1	0	-2.268909	-0.735714	-0.465298
8	8	0	1.972927	-0.085368	-0.100971
9	1	0	1.127888	0.371143	0.113468
10	1	0	2.245048	-0.474419	0.742773

Formaldehyde Solvated by Water

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.241228	0.494254	0.013393
2	1	0	2.299037	0.820902	0.037655
3	1	0	0.470084	1.284609	0.002307
4	8	0	0.943034	-0.681237	-0.000125
5	8	0	-1.814185	0.115833	-0.094922

6	1	0	-1.045262	-0.482165	-0.133729
7	1	0	-2.202023	-0.065638	0.773781

Acetone Solvated by Water

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.730791	-0.088416	-0.007396
2	8	0	-0.039022	-1.037920	-0.039672
3	8	0	-2.767069	-0.076152	-0.070656
4	1	0	-1.923404	-0.565253	-0.141216
5	1	0	-3.062380	-0.266807	0.832059
6	6	0	2.230137	-0.309795	0.032471
7	1	0	2.718425	0.220593	-0.794251
8	1	0	2.646869	0.099881	0.961367
9	1	0	2.454023	-1.376475	-0.028425
10	6	0	0.240939	1.345260	-0.008093
11	1	0	0.677204	1.899620	0.832181
12	1	0	0.576680	1.848642	-0.924181
13	1	0	-0.849892	1.370086	0.043201

Isomers of *N*-Methylcarbaminic Acid

N-Methylcarbaminic Acid, trans-trans, **1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.628206	-0.656642	-0.077414
2	1	0	-0.629332	-1.659752	0.033652
3	6	0	-1.883832	0.067924	0.036289
4	1	0	-2.130259	0.327996	1.074734
5	1	0	-1.830683	0.988895	-0.546947
6	1	0	-2.686563	-0.554057	-0.369022
7	6	0	0.614714	-0.106955	-0.007964
8	8	0	1.658651	-0.733769	0.035376
9	8	0	0.565333	1.257793	-0.013762
10	1	0	1.497115	1.535396	0.006624

N-Methylcarbaminic Acid, trans-cis, **2**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.627494	-0.611552	-0.000107
2	1	0	0.547669	-1.617613	0.000066
3	6	0	1.934834	0.013877	0.000047
4	1	0	2.509918	-0.264466	-0.891272
5	1	0	1.782362	1.094033	-0.000433
6	1	0	2.509428	-0.263725	0.891922

7	6	0	-0.524473	0.107481	-0.000015
8	8	0	-0.621758	1.322108	-0.000012
9	8	0	-1.606432	-0.729237	0.000038
10	1	0	-2.378485	-0.138481	0.000062

N-Methylcarbaminic Acid, cis-trans, **3**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.585412	-0.662958	-0.151101
2	1	0	-0.542260	-1.665853	-0.038846
3	6	0	-1.863586	-0.009914	0.079180
4	1	0	-1.938783	0.452964	1.073540
5	1	0	-2.068919	0.753388	-0.684412
6	1	0	-2.655541	-0.757016	-0.006736
7	6	0	0.655502	-0.074343	-0.015898
8	8	0	1.686693	-0.700794	0.069654
9	8	0	0.660144	1.289864	-0.004872
10	1	0	-0.222807	1.650202	-0.183780

N-Methylcarbaminic Acid, cis-cis, C_s-**4a**, (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.581066	-0.647799	-0.000008
2	1	0	-0.515791	-1.653952	0.000021
3	6	0	-1.901326	-0.036336	-0.000003
4	1	0	-2.042626	0.590605	0.886412
5	1	0	-2.042587	0.590684	-0.886367
6	1	0	-2.652828	-0.829317	-0.000057
7	6	0	0.537535	0.144212	0.000040
8	8	0	0.502885	1.354256	-0.000010
9	8	0	1.733941	-0.520270	-0.000010
10	1	0	1.609431	-1.482571	-0.000019

N-Methylcarbaminic Acid, cis-cis, C_1-**4b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.583319	-0.657545	-0.074056
2	1	0	-0.508835	-1.581314	0.332926
3	6	0	-1.898885	-0.034074	0.012513
4	1	0	-2.151086	0.281889	1.033437
5	1	0	-1.904984	0.848449	-0.628275
6	1	0	-2.652275	-0.742024	-0.343130
7	6	0	0.536727	0.148408	-0.001806
8	8	0	0.515055	1.357085	0.000056
9	8	0	1.720808	-0.535658	0.035391
10	1	0	1.586450	-1.461602	-0.224380

Isomers of *N*-Methylcarbaminic Acid, Aggregate with Formaldehyde

N-Methylcarbaminic Acid, trans-trans, Aggregate with Formaldehyde, **5**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.509273	0.664037	-0.021516
2	1	0	0.494670	0.831240	-0.008244
3	6	0	-1.430992	1.788003	0.004496
4	1	0	-2.143313	1.737612	-0.825419
5	1	0	-1.999126	1.830058	0.941388
6	1	0	-0.848141	2.706943	-0.091235
7	6	0	-0.874761	-0.634764	-0.003801
8	8	0	-0.112183	-1.596186	-0.002323
9	8	0	-2.231405	-0.788020	0.008869
10	1	0	-2.369850	-1.750404	0.013997
11	8	0	2.479688	0.780835	0.007661
12	6	0	2.851726	-0.376656	0.001017
13	1	0	2.133616	-1.213383	-0.009163
14	1	0	3.932416	-0.622843	0.005356

N-Methylcarbaminic Acid, trans-cis, Aggregate with Formaldehyde, **6**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.585208	0.656602	0.000022
2	1	0	0.426851	0.755944	0.000121
3	6	0	-1.425719	1.837550	-0.000004
4	1	0	-1.244408	2.451654	-0.890353
5	1	0	-2.466556	1.510728	-0.000254
6	1	0	-1.244783	2.451455	0.890562
7	6	0	-1.107621	-0.588725	0.000005
8	8	0	-2.287534	-0.898969	-0.000069
9	8	0	-0.107636	-1.537609	0.000073
10	1	0	-0.584577	-2.384884	0.000049
11	8	0	2.441496	0.781007	0.000029
12	6	0	2.943894	-0.322883	-0.000058
13	1	0	2.331883	-1.240887	-0.000056
14	1	0	4.044119	-0.451307	-0.000142

N-Methylcarbaminic Acid, cis-trans, Aggregate with Formaldehyde, **7**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.517095	0.634814	-0.000047
2	1	0	-0.488292	0.802165	-0.000032
3	6	0	1.420527	1.768310	0.000017
4	1	0	2.059947	1.795655	0.894771
5	1	0	2.060051	1.795663	-0.894662

6	1	0	0.824304	2.683194	-0.000018
7	6	0	0.871690	-0.683594	-0.000009
8	8	0	0.073885	-1.604169	-0.000002
9	8	0	2.210153	-0.949640	0.000017
10	1	0	2.733795	-0.132922	-0.000011
11	8	0	-2.454980	0.800503	0.000003
12	6	0	-2.851306	-0.349562	0.000010
13	1	0	-2.150428	-1.200360	0.000001
14	1	0	-3.936975	-0.571575	0.000027

N-Methylcarbaminic Acid, cis-cis, Aggregate with Formaldehyde, C_s-**8a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.859108	0.693357	-0.000212
2	1	0	-0.076215	1.071393	0.000352
3	6	0	1.992050	1.601894	0.000066
4	1	0	2.618579	1.453035	0.886305
5	1	0	2.619969	1.451458	-0.884890
6	1	0	1.616179	2.628289	-0.001139
7	6	0	1.068608	-0.662583	-0.000022
8	8	0	2.172504	-1.167639	-0.000047
9	8	0	-0.060252	-1.423966	0.000114
10	1	0	-0.859123	-0.862295	0.000075
11	8	0	-2.287156	0.428980	0.000081
12	6	0	-3.470353	0.164491	-0.000066
13	1	0	-3.838366	-0.877250	-0.000246
14	1	0	-4.237376	0.960058	-0.000029

N-Methylcarbaminic Acid, cis-cis, Aggregate with Formaldehyde, C_1-**8b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.868902	0.694854	-0.068063
2	1	0	0.061083	1.059750	0.082377
3	6	0	-1.984584	1.619461	0.012920
4	1	0	-1.831096	2.460013	-0.672529
5	1	0	-2.885019	1.077484	-0.278352
6	1	0	-2.129247	2.013860	1.028514
7	6	0	-1.075100	-0.665510	-0.005114
8	8	0	-2.168622	-1.191731	-0.003239
9	8	0	0.062832	-1.410497	0.028626
10	1	0	0.855900	-0.841147	-0.004315
11	8	0	2.291264	0.433623	0.044538
12	6	0	3.469333	0.156194	-0.027190
13	1	0	3.821074	-0.885101	-0.139924
14	1	0	4.247932	0.939147	0.017577

Isomers of *N*-Methylcarbaminic Acid, Aggregate with Acetone

N-Methylcarbaminic Acid, trans-trans, Aggregate with Acetone, **9b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.382501	0.653343	0.032506
2	1	0	-0.364677	0.694403	0.028946
3	6	0	-2.142431	1.891519	0.062802
4	1	0	-2.740856	2.025404	-0.845971
5	1	0	-2.818214	1.928404	0.924381
6	1	0	-1.433537	2.719199	0.138853
7	6	0	-1.922257	-0.580379	-0.033614
8	8	0	-1.302749	-1.638192	-0.075585
9	8	0	-3.289507	-0.544483	-0.047605
10	1	0	-3.555837	-1.478475	-0.091990
11	8	0	1.567311	0.967986	-0.007621
12	6	0	2.421782	0.092964	0.008511
13	6	0	3.890451	0.452561	-0.112934
14	1	0	4.015380	1.537014	-0.098165
15	1	0	4.470289	-0.002874	0.698903
16	1	0	4.293200	0.053042	-1.052607
17	6	0	2.080501	-1.373146	0.156744
18	1	0	1.005198	-1.542953	0.053841
19	1	0	2.632720	-1.974611	-0.575565
20	1	0	2.405115	-1.715555	1.149265

N-Methylcarbaminic Acid, trans-cis, Aggregate with Acetone, **10b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.458302	0.658579	0.015158
2	1	0	-0.441578	0.616069	-0.000836
3	6	0	-2.112101	1.951433	0.048852
4	1	0	-1.872024	2.541400	-0.844328
5	1	0	-3.189803	1.785668	0.085166
6	1	0	-1.807762	2.522365	0.934239
7	6	0	-2.163309	-0.491875	-0.019906
8	8	0	-3.377601	-0.619238	-0.017854
9	8	0	-1.321397	-1.581059	-0.058652
10	1	0	-1.921343	-2.345680	-0.079396
11	8	0	1.531086	0.895594	-0.029125
12	6	0	2.444922	0.085732	0.001971
13	6	0	3.889016	0.544747	-0.060719
14	1	0	3.936314	1.635312	-0.061177
15	1	0	4.457946	0.147253	0.788591
16	1	0	4.365837	0.157988	-0.970364
17	6	0	2.200345	-1.405268	0.107070
18	1	0	1.132829	-1.626277	0.049313
19	1	0	2.738399	-1.938758	-0.686309
20	1	0	2.599356	-1.776388	1.060418

N-Methylcarbaminic Acid, cis-trans, Aggregate with Acetone, **11b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.381339	0.619584	0.058918
2	1	0	-0.361831	0.647451	0.054251
3	6	0	-2.100364	1.877454	0.046107
4	1	0	-2.686190	2.021409	-0.874163
5	1	0	-2.769966	1.987108	0.912488
6	1	0	-1.369511	2.687245	0.098329
7	6	0	-1.929864	-0.626415	-0.030028
8	8	0	-1.283818	-1.657501	-0.074208
9	8	0	-3.295405	-0.683333	-0.064580
10	1	0	-3.686078	0.202238	0.000751
11	8	0	1.548238	0.966865	0.007925
12	6	0	2.409830	0.097720	0.009943
13	6	0	3.874175	0.471007	-0.118625
14	1	0	3.990896	1.556177	-0.092124
15	1	0	4.464072	0.010421	0.682927
16	1	0	4.272325	0.085686	-1.066147
17	6	0	2.081027	-1.371616	0.147096
18	1	0	1.006851	-1.550280	0.046794
19	1	0	2.636005	-1.962714	-0.591457
20	1	0	2.411865	-1.718975	1.135878

N-Methylcarbaminic Acid, cis-cis, Aggregate with Acetone, **12b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.661825	0.763689	0.001608
2	1	0	0.824436	1.150872	-0.411140
3	6	0	2.738051	1.672393	0.349831
4	1	0	2.373086	2.455265	1.023866
5	1	0	3.508895	1.091395	0.857486
6	1	0	3.185904	2.148667	-0.533535
7	6	0	1.886809	-0.591698	-0.098449
8	8	0	2.921046	-1.139014	0.224801
9	8	0	0.829334	-1.304219	-0.572653
10	1	0	0.065177	-0.716390	-0.761439
11	8	0	-1.374046	0.430391	-0.735503
12	6	0	-2.338878	0.094182	-0.056991
13	6	0	-3.543796	0.998835	0.066081
14	1	0	-3.444830	1.854507	-0.604185
15	1	0	-4.465273	0.448905	-0.159237
16	1	0	-3.632288	1.354467	1.100771
17	6	0	-2.380279	-1.229300	0.673146
18	1	0	-1.390496	-1.689299	0.699655
19	1	0	-2.767346	-1.104037	1.690553
20	1	0	-3.072162	-1.903909	0.151082

Isomers of MgL_2 Complexes of *N*-Methylcarbaminic Acid

N-Methylcarbaminic Acid, trans-trans **13a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.404985	-1.548817	-0.871428
2	8	0	2.275774	-1.068313	1.288939
3	1	0	3.454674	-2.569929	0.555206
4	8	0	1.688256	1.785529	-1.026094
5	8	0	0.441841	1.793756	0.801595
6	1	0	0.964214	3.504856	-0.201491
7	8	0	-0.673593	-0.637326	-0.460080
8	8	0	-2.024021	0.864962	0.596359
9	1	0	-1.150746	1.334256	0.744878
10	6	0	2.740364	-1.761724	0.330886
11	6	0	1.031457	2.406954	-0.152200
12	6	0	-1.805825	-0.245799	-0.087103
13	7	0	-2.908211	-0.952154	-0.382746
14	1	0	-2.731250	-1.827698	-0.854564
15	6	0	-4.259872	-0.626069	0.052683
16	1	0	-4.392660	0.456503	0.049508
17	1	0	-4.969892	-1.072617	-0.647130
18	1	0	-4.465330	-1.004088	1.061051
19	12	0	1.208816	-0.026225	-0.127347

Complex *N*-Methylcarbaminic Acid, trans-trans, **13b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.056565	1.784599	0.674391
2	8	0	1.382569	1.909770	-1.094164
3	1	0	0.362521	3.521017	-0.369020
4	8	0	2.207814	-0.751201	1.437192
5	8	0	2.670215	-1.212578	-0.681275
6	1	0	3.697420	-2.037646	0.881676
7	8	0	-0.524213	-0.916326	-0.600447
8	8	0	-2.603498	-1.769731	-0.636691
9	1	0	-2.085591	-2.461818	-1.084965
10	6	0	0.592758	2.447916	-0.270604
11	6	0	2.890769	-1.360991	0.556394
12	6	0	-1.735431	-0.800982	-0.305131
13	7	0	-2.278204	0.234882	0.328601
14	1	0	-1.621054	0.977207	0.583233
15	6	0	-3.689304	0.335289	0.683988
16	1	0	-3.981984	-0.462513	1.373659
17	1	0	-3.843756	1.298818	1.171976
18	1	0	-4.324064	0.280865	-0.205463
19	12	0	1.156297	0.096354	-0.119269

Complex *N*-Methylcarbaminic Acid, trans-cis, **14a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.866470	-1.897255	-0.798787
2	8	0	2.080466	-1.215015	1.299654
3	1	0	2.854704	-2.983288	0.623877
4	8	0	1.823427	1.489183	-1.229490
5	8	0	0.774239	1.905813	0.673042
6	1	0	1.530236	3.383632	-0.531827
7	8	0	-0.903184	-0.358217	-0.230845
8	8	0	-1.843193	1.487346	0.722400
9	1	0	-0.887557	1.781082	0.767732
10	6	0	2.289532	-2.068998	0.382221
11	6	0	1.384158	2.303360	-0.377288
12	6	0	-1.901988	0.284662	0.167927
13	7	0	-3.151655	-0.192571	0.063323
14	1	0	-3.885930	0.402475	0.421471
15	6	0	-3.485354	-1.493319	-0.495220
16	1	0	-2.564140	-1.963682	-0.838130
17	1	0	-3.953200	-2.131642	0.261864
18	1	0	-4.168911	-1.382682	-1.343352
19	12	0	1.086041	-0.100581	-0.113210

Complex *N*-Methylcarbaminic Acid, trans-cis, **14b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.136993	-1.669128	1.064139
2	8	0	-1.921841	-1.667879	-1.007648
3	1	0	-1.995780	-3.313302	0.201577
4	8	0	-1.034376	1.675510	1.101320
5	8	0	-1.853253	1.753761	-0.955712
6	1	0	-1.830406	3.375135	0.287660
7	8	0	0.877730	-0.024304	-0.846832
8	8	0	3.024784	0.013415	-1.523293
9	1	0	2.551766	0.032872	-2.373860
10	6	0	-1.696766	-2.258155	0.090148
11	6	0	-1.582391	2.309896	0.149872
12	6	0	2.086323	-0.019199	-0.559941
13	7	0	2.596917	-0.047753	0.671524
14	1	0	3.604153	-0.030699	0.744786
15	6	0	1.774624	-0.079767	1.883272
16	1	0	2.446985	-0.139502	2.740337
17	1	0	1.163443	0.823788	1.961993
18	1	0	1.115851	-0.952513	1.878937
19	12	0	-1.031131	0.014238	-0.181500

Complex *N*-Methylcarbaminic Acid, cis-trans, **15a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.563458	2.068629	-0.696641
2	8	0	-0.214821	1.652416	1.014353
3	1	0	-0.675605	3.546317	0.397005
4	8	0	-2.491187	-1.192995	-1.072657
5	8	0	-2.238511	-1.123328	1.129040
6	1	0	-3.532070	-2.405905	0.200920
7	8	0	0.632685	-0.500180	-0.851791
8	8	0	1.640635	-1.009553	1.064411
9	1	0	2.448687	-0.811991	1.565648
10	6	0	-0.811576	2.461582	0.246645
11	6	0	-2.782903	-1.604945	0.087212
12	6	0	1.675962	-0.536936	-0.187833
13	7	0	2.863632	-0.152476	-0.697388
14	1	0	2.809074	0.234896	-1.629234
15	6	0	4.151700	-0.224244	-0.022452
16	1	0	4.352185	-1.239612	0.338736
17	1	0	4.931933	0.033140	-0.740121
18	1	0	4.218858	0.485298	0.812889
19	12	0	-1.176695	0.124379	-0.124940

Complex *N*-Methylcarbaminic Acid, cis-trans, **15b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.062153	1.767390	0.685465
2	8	0	1.395857	1.913608	-1.075819
3	1	0	0.387011	3.519487	-0.325709
4	8	0	2.141715	-0.807450	1.441233
5	8	0	2.723887	-1.179213	-0.665157
6	1	0	3.674669	-2.056195	0.917443
7	8	0	-0.525233	-0.898330	-0.659458
8	8	0	-2.533162	-1.815649	-0.728190
9	1	0	-3.453006	-1.656426	-0.461201
10	6	0	0.607675	2.442589	-0.246199
11	6	0	2.878686	-1.375077	0.575888
12	6	0	-1.726194	-0.810564	-0.353907
13	7	0	-2.252794	0.227433	0.316475
14	1	0	-1.576789	0.956953	0.568189
15	6	0	-3.641190	0.350978	0.731259
16	1	0	-3.940858	-0.459037	1.409244
17	1	0	-3.750935	1.291429	1.273176
18	1	0	-4.325227	0.382266	-0.127578
19	12	0	1.159926	0.078257	-0.141310

Complex *N*-Methylcarbaminic Acid, cis-cis, **16a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.183852	2.114786	-0.760108
2	8	0	-0.237401	1.617014	1.182760
3	1	0	-0.429954	3.534329	0.499152
4	8	0	-2.245636	-1.082995	-1.325889
5	8	0	-2.430319	-1.008994	0.882222
6	1	0	-3.598208	-2.210906	-0.288798
7	8	0	0.812389	-0.587733	-0.530681
8	8	0	1.383149	-1.133597	1.550135
9	1	0	2.044480	-0.879431	2.214731
10	6	0	-0.609793	2.461003	0.317094
11	6	0	-2.788996	-1.463179	-0.248587
12	6	0	1.704199	-0.706107	0.316864
13	7	0	3.000472	-0.441243	0.059485
14	1	0	3.700451	-0.769041	0.710647
15	6	0	3.449744	0.012181	-1.254918
16	1	0	4.356261	0.608833	-1.131572
17	1	0	3.654247	-0.831142	-1.923691
18	1	0	2.667796	0.630270	-1.696207
19	12	0	-1.059662	0.152879	-0.130906

Complex *N*-Methylcarbaminic Acid, cis-cis, **16b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.636184	1.647336	1.188547
2	8	0	1.769241	1.963896	-0.688920
3	1	0	1.390497	3.467968	0.640219
4	8	0	1.405373	-1.612193	0.937351
5	8	0	2.104642	-1.396906	-1.154045
6	1	0	2.448477	-3.075252	-0.041501
7	8	0	-0.864537	-0.141155	-0.871997
8	8	0	-2.924671	0.217699	-1.581440
9	1	0	-3.850271	0.121168	-1.304597
10	6	0	1.269377	2.400803	0.390987
11	6	0	2.004177	-2.067404	-0.086327
12	6	0	-2.064373	-0.089415	-0.591815
13	7	0	-2.574814	-0.349341	0.627628
14	1	0	-3.543971	-0.125446	0.805043
15	6	0	-1.732112	-0.644128	1.792935
16	1	0	-2.368770	-1.081433	2.564551
17	1	0	-0.960252	-1.365606	1.517750
18	1	0	-1.249928	0.261516	2.171780
19	12	0	1.023804	0.101161	-0.201440

Isomers of MgL_2 Complexes of *N*-Methylcarbaminic Acid, Aggr. with FA

17a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.671640	2.135025	-0.357731
2	8	0	-2.375770	1.138313	1.493756
3	1	0	-2.563426	3.148647	1.179721
4	8	0	-2.519636	-1.062990	-1.413516
5	8	0	-1.606415	-2.063420	0.337079
6	1	0	-2.624054	-3.079900	-1.124622
7	8	0	0.497619	-0.030035	-0.068238
8	8	0	1.077960	-2.176918	0.428123
9	1	0	0.086963	-2.287387	0.424462
10	6	0	-2.217169	2.179608	0.785812
11	6	0	-2.266441	-2.106431	-0.755093
12	6	0	1.369731	-0.910866	0.160563
13	7	0	2.667974	-0.612336	0.143900
14	1	0	2.881755	0.363200	-0.073609
15	6	0	3.734518	-1.573250	0.388787
16	1	0	3.754871	-2.351447	-0.381309
17	1	0	4.683513	-1.034508	0.373229
18	1	0	3.613663	-2.053399	1.364383
19	12	0	-1.487635	0.073596	-0.022974
20	8	0	2.973421	2.243449	-0.512583
21	6	0	1.947210	2.883324	-0.638039
22	1	0	1.982353	3.956062	-0.908685
23	1	0	0.948765	2.440231	-0.492480

17b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.192741	-1.309916	-1.505322
2	8	0	1.165820	-2.247278	0.219424
3	1	0	2.002425	-3.331591	-1.303526
4	8	0	1.926792	1.904902	-0.238300
5	8	0	2.401501	0.697076	1.559560
6	1	0	2.944339	2.657102	1.369675
7	8	0	-0.589923	0.214860	-0.094059
8	8	0	-2.830567	0.158455	0.055321
9	1	0	-2.682489	1.125979	-0.140833
10	6	0	1.795747	-2.334846	-0.881872
11	6	0	2.443848	1.787511	0.913436
12	6	0	-1.650029	-0.437071	0.099721
13	7	0	-1.674571	-1.746419	0.358123
14	1	0	-0.762829	-2.204056	0.378050
15	6	0	-2.894542	-2.509449	0.588252
16	1	0	-3.526619	-2.529941	-0.305633
17	1	0	-2.609794	-3.531220	0.845218
18	1	0	-3.472899	-2.083708	1.413349
19	12	0	1.375706	-0.119592	-0.028561

20	8	0	-2.434982	2.805193	-0.493260
21	6	0	-1.317412	3.282085	-0.584101
22	1	0	-0.402541	2.688441	-0.434804
23	1	0	-1.192794	4.353307	-0.825157

17c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.247676	-0.534571	-1.961346
2	8	0	-2.485491	0.828014	-0.232281
3	1	0	-3.609642	0.987126	-1.936156
4	8	0	-1.158701	-2.546370	0.642051
5	8	0	-0.544331	-0.767742	1.816518
6	1	0	-0.703904	-2.636384	2.630765
7	8	0	0.755143	-0.221820	-0.906778
8	8	0	2.121177	1.186042	0.242546
9	1	0	1.278296	1.708660	0.392257
10	6	0	-2.811734	0.446385	-1.402369
11	6	0	-0.798320	-2.004373	1.732225
12	6	0	1.884226	0.104592	-0.472685
13	7	0	2.970610	-0.642617	-0.730183
14	1	0	2.802559	-1.445823	-1.318664
15	6	0	4.333238	-0.298047	-0.345538
16	1	0	4.344499	0.080753	0.677955
17	1	0	4.945248	-1.201031	-0.395962
18	1	0	4.762961	0.462705	-1.007538
19	12	0	-1.060056	-0.699899	-0.254397
20	8	0	-0.011256	2.766326	0.585251
21	6	0	-1.004415	2.499062	1.242105
22	1	0	-1.864915	3.186758	1.255907
23	1	0	-1.077597	1.589594	1.855378

17d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.032192	-0.706088	-1.823581
2	8	0	3.051276	-0.126789	0.058846
3	1	0	4.052129	-0.850379	-1.570396
4	8	0	0.991471	2.252836	-0.531017
5	8	0	0.194892	1.387825	1.347477
6	1	0	0.345284	3.407091	1.018257
7	8	0	-0.971502	-0.256127	-0.862957
8	8	0	-2.255731	0.493976	0.862708
9	1	0	-1.374614	0.868040	1.165253
10	6	0	3.080653	-0.570697	-1.127874
11	6	0	0.509461	2.394714	0.613426
12	6	0	-2.072628	-0.144725	-0.284291
13	7	0	-3.187821	-0.692711	-0.803630
14	1	0	-3.056466	-1.124446	-1.707184
15	6	0	-4.531998	-0.534766	-0.268533

16	1	0	-5.007116	0.391285	-0.615357
17	1	0	-5.139709	-1.385506	-0.586628
18	1	0	-4.489768	-0.519353	0.821212
19	12	0	0.944266	0.139524	-0.269947
20	8	0	0.717265	-1.575161	1.115300
21	6	0	1.606406	-1.982042	1.842602
22	1	0	2.623562	-1.569801	1.778569
23	1	0	1.399976	-2.780921	2.574849

17e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.372329	-0.518793	-1.850957
2	8	0	-2.009993	1.284427	-0.617427
3	1	0	-3.144247	1.313243	-2.320968
4	8	0	-1.898742	-1.937650	1.250568
5	8	0	-0.626196	-0.242232	1.902058
6	1	0	-1.390415	-1.622643	3.203034
7	8	0	0.610468	-1.012507	-0.833131
8	8	0	2.716112	-1.797342	-0.885546
9	1	0	2.204970	-2.542067	-1.248295
10	6	0	-2.533497	0.713583	-1.626900
11	6	0	-1.307184	-1.278350	2.158898
12	6	0	1.826264	-0.830511	-0.599956
13	7	0	2.359080	0.273747	-0.093815
14	1	0	1.725000	1.050908	0.117269
15	6	0	3.785933	0.457403	0.148203
16	1	0	4.362525	0.322625	-0.771766
17	1	0	3.929664	1.475800	0.512157
18	1	0	4.154452	-0.246710	0.900741
19	12	0	-1.204079	-0.571996	-0.122488
20	8	0	0.851875	2.696579	0.278139
21	6	0	-0.212832	2.858258	0.845540
22	1	0	-0.790205	3.790018	0.705814
23	1	0	-0.638025	2.104398	1.524226

17f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.247233	-0.690229	-1.603090
2	8	0	2.977845	0.108051	0.332463
3	1	0	4.225688	-0.636791	-1.105287
4	8	0	0.773205	2.235160	-0.689516
5	8	0	-0.085417	1.428209	1.189070
6	1	0	-0.097362	3.422226	0.719299
7	8	0	-0.849441	-0.494562	-1.091991
8	8	0	-2.974166	-1.174887	-1.378202
9	1	0	-2.515291	-1.587946	-2.130999
10	6	0	3.187775	-0.413867	-0.803161
11	6	0	0.190764	2.403108	0.408843

12	6	0	-2.031426	-0.495484	-0.698039
13	7	0	-2.487540	0.141150	0.381558
14	1	0	-1.782106	0.683038	0.888655
15	6	0	-3.876770	0.129629	0.819507
16	1	0	-4.219782	-0.889831	1.021594
17	1	0	-3.943453	0.712797	1.739679
18	1	0	-4.536533	0.576596	0.068544
19	12	0	0.911785	0.166418	-0.256007
20	8	0	0.657476	-1.497019	1.190570
21	6	0	1.474681	-1.758550	2.055898
22	1	0	2.439824	-1.234094	2.101073
23	1	0	1.256348	-2.537859	2.805907

18a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.207625	-1.452163	-0.367199
2	8	0	2.852903	-0.533108	1.618946
3	1	0	4.191232	-2.050784	1.322020
4	8	0	2.297809	1.699081	-1.300447
5	8	0	0.906553	2.004065	0.393439
6	1	0	1.418237	3.497897	-0.914822
7	8	0	0.051271	-0.726960	-0.396568
8	8	0	-1.478022	0.844478	0.219848
9	1	0	-0.649279	1.393975	0.320531
10	6	0	3.447070	-1.373159	0.873600
11	6	0	1.538983	2.441846	-0.626383
12	6	0	-1.137529	-0.378354	-0.191748
13	7	0	-2.178762	-1.192569	-0.370179
14	1	0	-3.103449	-0.809536	-0.167630
15	6	0	-2.053231	-2.575216	-0.802072
16	1	0	-2.412629	-3.256554	-0.023220
17	1	0	-2.635694	-2.741912	-1.714084
18	1	0	-1.003123	-2.785552	-1.004004
19	12	0	1.848580	0.087967	-0.066535
20	8	0	-4.796132	0.036454	0.294389
21	6	0	-4.736292	1.163390	0.740743
22	1	0	-5.651671	1.708804	1.038449
23	1	0	-3.775311	1.690211	0.868329

18b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.721939	-1.136677	-1.865370
2	8	0	0.564279	-2.412334	-0.472257
3	1	0	1.128705	-3.032883	-2.338679
4	8	0	2.450919	1.120464	0.564469
5	8	0	1.812923	-0.464016	1.975330
6	1	0	3.055304	1.064872	2.518142
7	8	0	-0.622202	0.437125	-0.119786

8	8	0	-2.740294	1.173898	0.101496
9	1	0	-2.887301	0.219782	0.357632
10	6	0	1.138039	-2.224902	-1.588844
11	6	0	2.462934	0.592080	1.717863
12	6	0	-1.458923	1.362410	-0.177288
13	7	0	-1.162369	2.622590	-0.523455
14	1	0	-1.944491	3.258914	-0.585974
15	6	0	0.162668	3.062368	-0.948614
16	1	0	0.188363	4.153036	-0.905555
17	1	0	0.930900	2.662820	-0.283121
18	1	0	0.381632	2.742269	-1.974194
19	12	0	1.158760	-0.441632	0.006613
20	8	0	-3.286216	-1.383527	0.812931
21	6	0	-2.542500	-2.330225	0.620939
22	1	0	-1.563753	-2.236169	0.125250
23	1	0	-2.842013	-3.341019	0.952483

Isomers of MgL_2 Complexes of *N*-Methylcarbaminic Acid, Aggr. with Acetone

21a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.719176	-2.563537	0.141327
2	8	0	-2.096185	-1.978560	-1.494648
3	1	0	-1.191586	-3.808690	-1.412102
4	8	0	-2.935603	-0.390643	1.667232
5	8	0	-3.014633	1.006897	-0.048077
6	1	0	-4.196207	1.212385	1.614719
7	8	0	-0.094589	0.513283	-0.044866
8	8	0	-0.890263	2.623675	-0.369727
9	1	0	-1.761453	2.147869	-0.281819
10	6	0	-1.330151	-2.822792	-0.939717
11	6	0	-3.412919	0.630434	1.104549
12	6	0	0.095841	1.744016	-0.237207
13	7	0	1.325735	2.248276	-0.326885
14	1	0	2.087322	1.584891	-0.157765
15	6	0	1.616067	3.664681	-0.499286
16	1	0	1.316473	4.248530	0.378210
17	1	0	2.692571	3.771989	-0.644557
18	1	0	1.096683	4.063793	-1.374856
19	12	0	-1.666547	-0.693844	0.058051
20	8	0	3.373285	0.339749	0.427257
21	6	0	3.343677	-0.873863	0.265686
22	6	0	4.115771	-1.791724	1.189791
23	1	0	4.575059	-1.216420	1.995684
24	1	0	3.449877	-2.556607	1.607631
25	1	0	4.894575	-2.321922	0.626982
26	6	0	2.538284	-1.526225	-0.833403
27	1	0	1.621204	-1.953669	-0.405360
28	1	0	2.254686	-0.790819	-1.588909
29	1	0	3.097118	-2.347198	-1.296735

21b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.927093	-0.522992	-0.084230
2	8	0	-2.107080	-1.640683	1.645246
3	1	0	-4.027993	-0.955162	1.587472
4	8	0	-0.657691	-2.661785	-1.487054
5	8	0	0.908442	-2.354320	0.050939
6	1	0	1.063454	-3.759781	-1.428552
7	8	0	-0.094597	0.547921	-0.081651
8	8	0	0.404755	2.741376	-0.101564
9	1	0	1.300248	2.364680	0.150702
10	6	0	-3.057935	-1.036798	1.070957
11	6	0	0.461540	-2.957059	-0.971828
12	6	0	-0.462817	1.746721	-0.187424
13	7	0	-1.731895	2.106106	-0.406854
14	1	0	-2.405069	1.339958	-0.399448
15	6	0	-2.187151	3.487809	-0.484167
16	1	0	-1.576778	4.053247	-1.192629
17	1	0	-3.221873	3.485090	-0.832096
18	1	0	-2.139596	3.985911	0.490905
19	12	0	-0.907196	-1.262528	0.009821
20	6	0	3.110163	0.579608	0.320666
21	8	0	2.645451	1.602963	0.816035
22	6	0	3.002250	0.275433	-1.153751
23	1	0	2.416829	-0.642108	-1.277491
24	1	0	2.519509	1.094459	-1.690021
25	1	0	3.996988	0.091261	-1.576998
26	6	0	3.783482	-0.456408	1.184632
27	1	0	3.885049	-0.091038	2.208035
28	1	0	3.159897	-1.360838	1.172768
29	1	0	4.764271	-0.733766	0.781199