New Jouranl of Chemistry

Electronic Supplementary Information

Theoretical investigation of the structures, stabilities, and vibrational and rotational spectroscopic parameters of linear HOMgNC and HMgNCO molecules by density functional theory and coupled-cluster method

Jie Bai, Hai-Tao Yu*

School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, P. R. China

E-mail: yuhaitao@hlju.edu.cn

Table of Contents

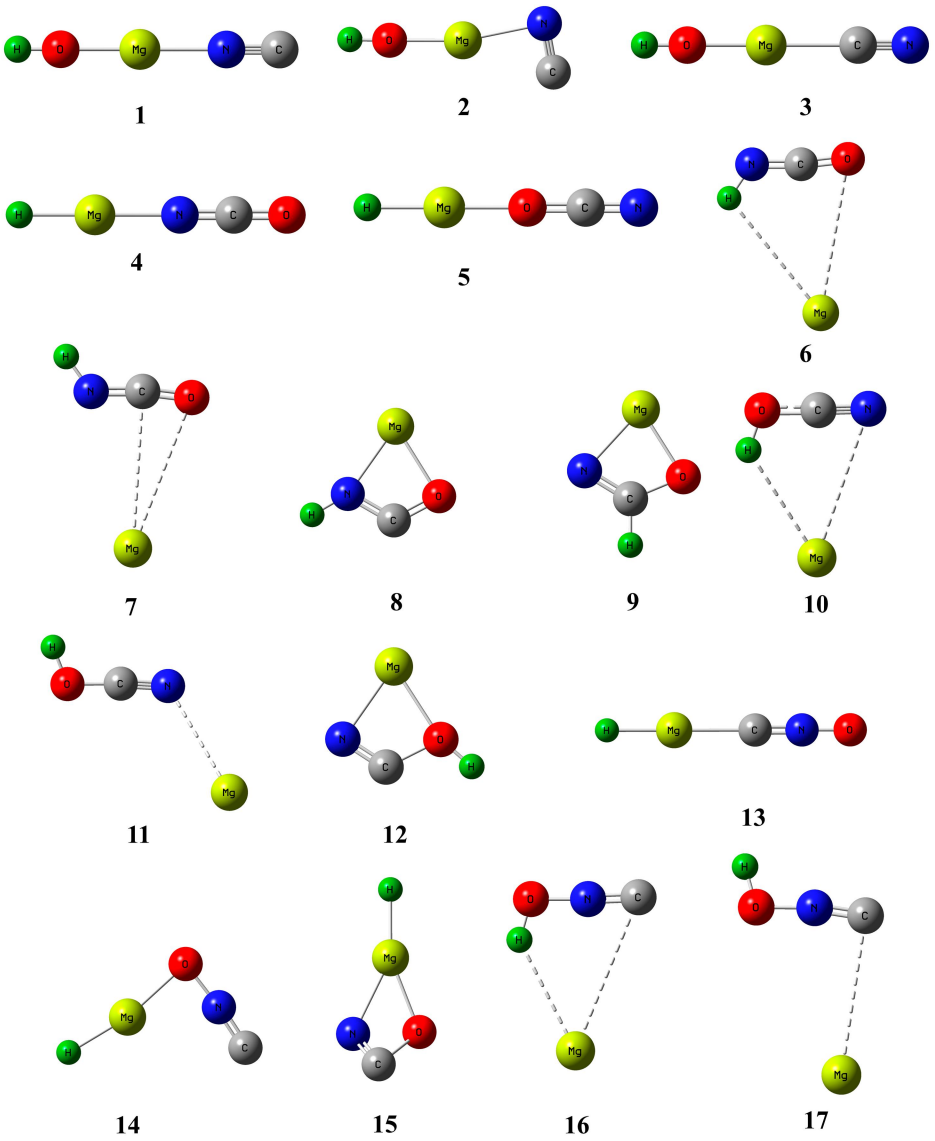


Figure S1 Structures of the singlet isomers for the [H,Mg,N,C,O] system optimized at the M06-2X/*aug-cc-p*VTZ level of theory.

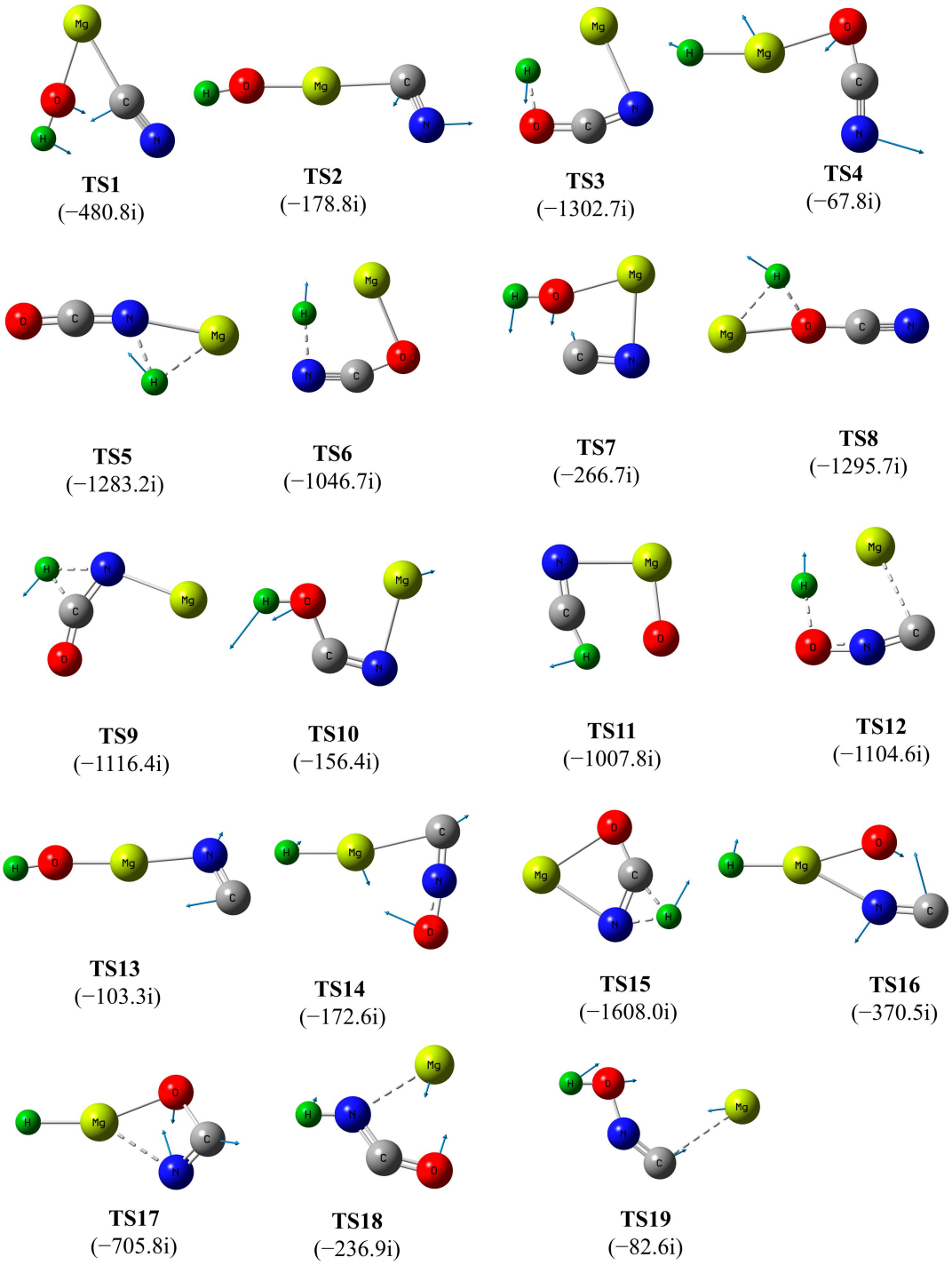


Figure S2 Structures of the singlet transition states for the [H,Mg,N,C,O] system optimized at the M06-2X/*aug-cc-p*VTZ level of theory.

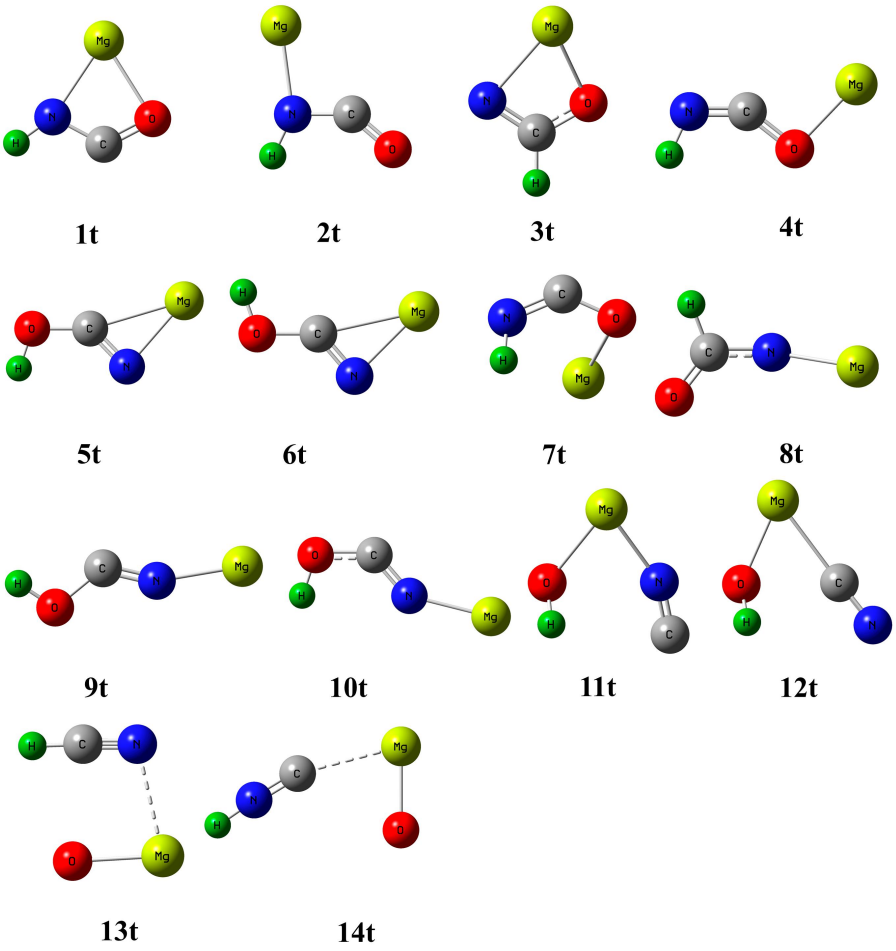


Figure S3 Structures of the triplet isomers for the [H,Mg,N,C,O] system optimized at the M06-2X/*aug-cc-p*VTZ level of theory.

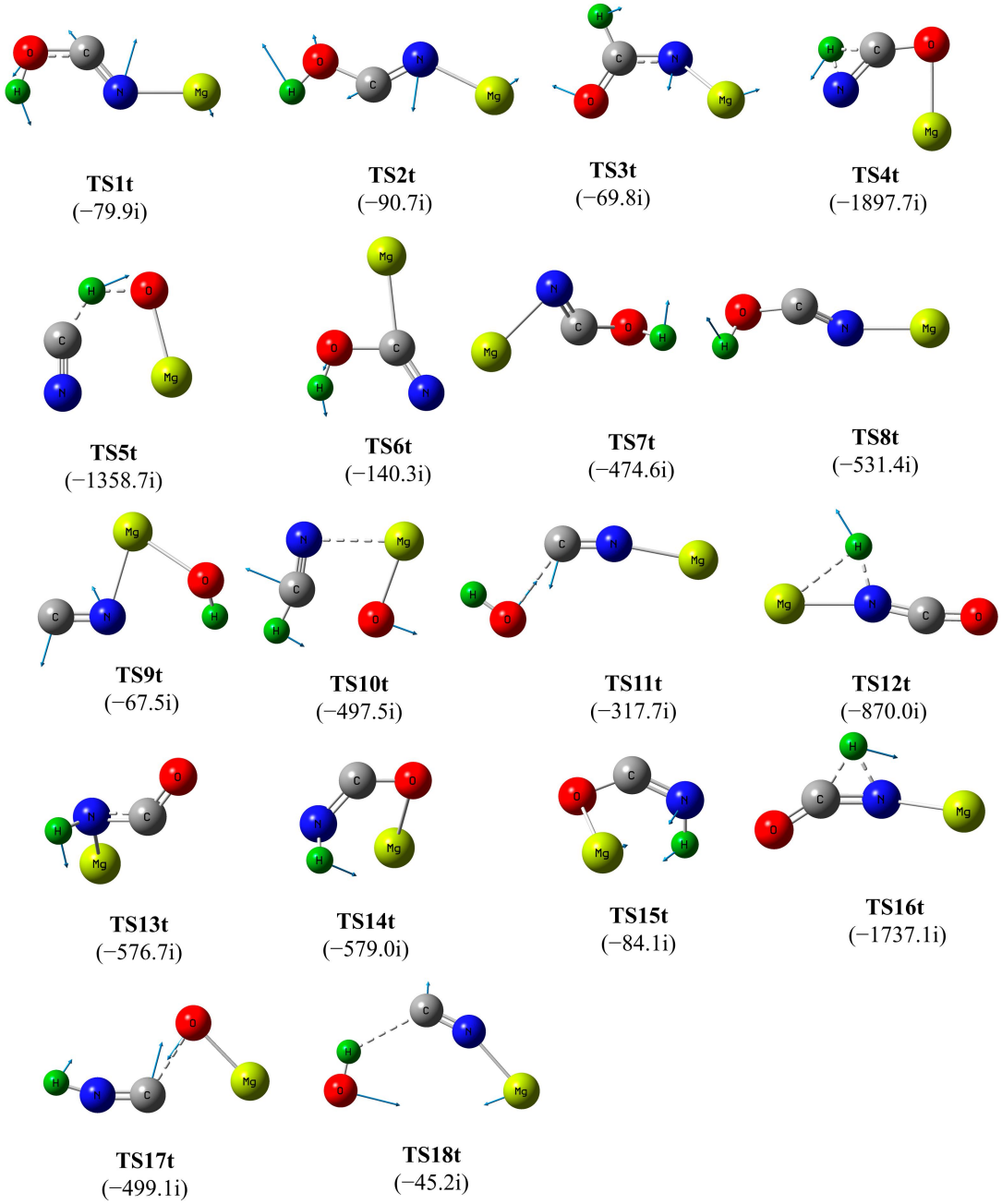


Figure S4 Structures of the triplet transition states for the [H,Mg,N,C,O] system optimized at the M06-2X/*aug-cc-p*VTZ level of theory.

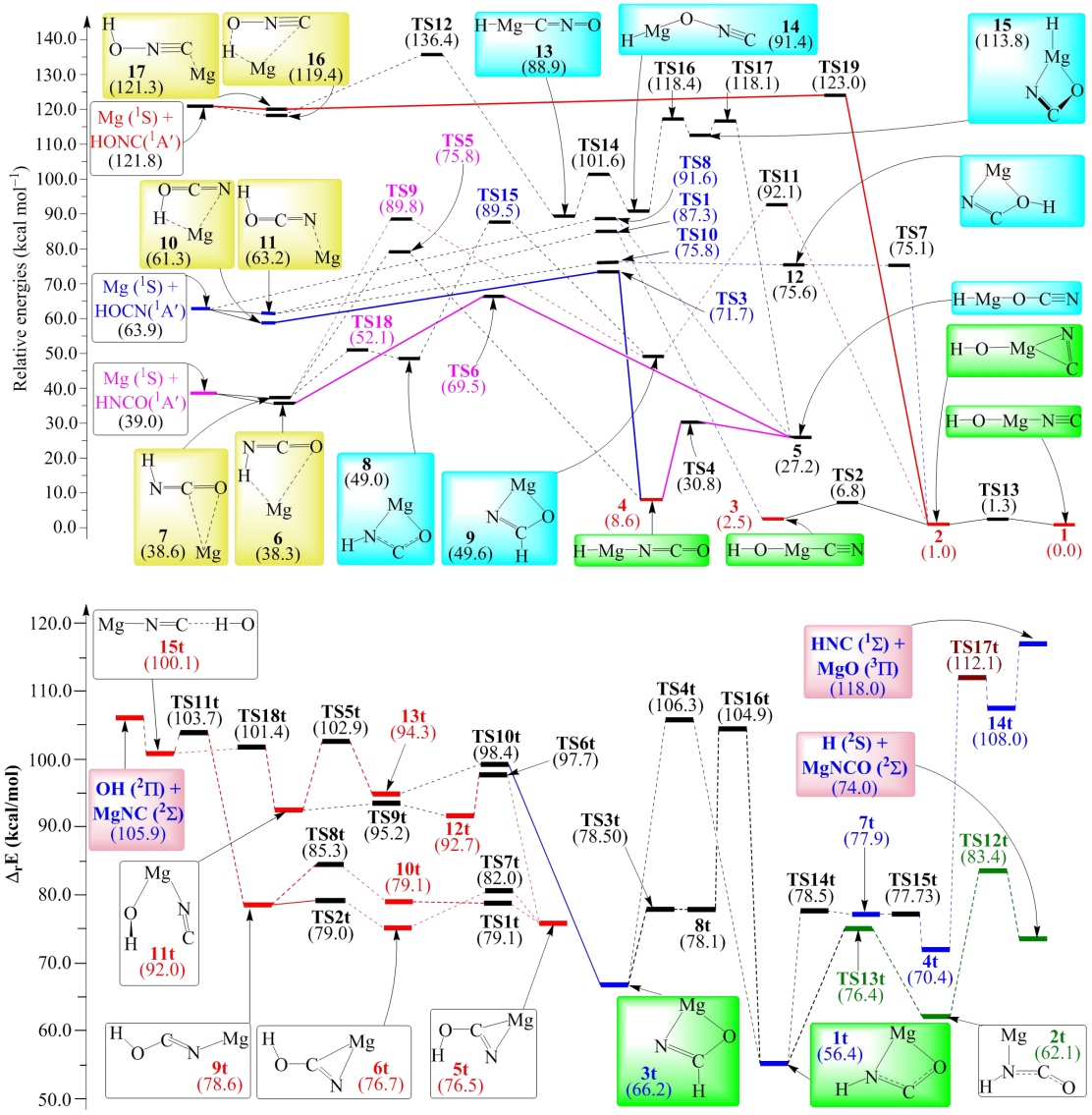


Figure S5 Singlet and triplet reaction potential energy profiles of the [H,Mg,N,C,O] system constructed at the M06-2X/*aug-cc-p*VTZ level of theory.

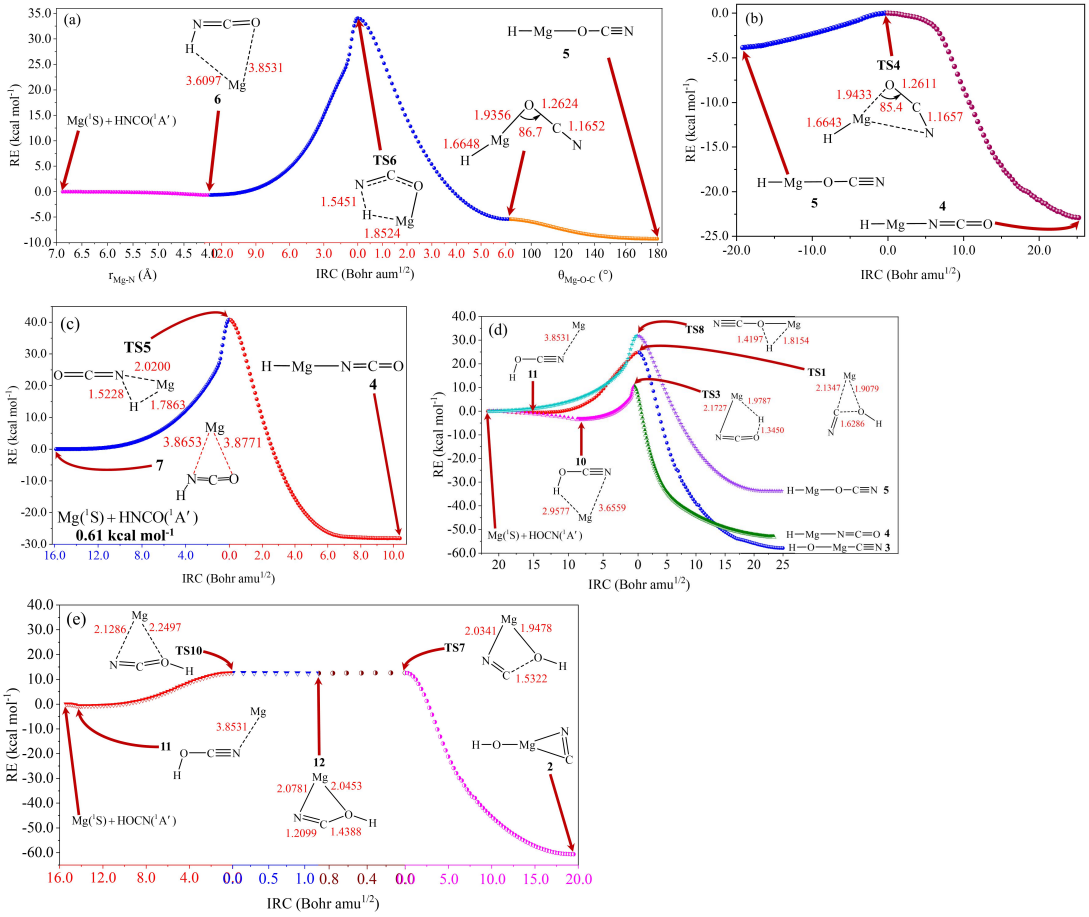


Figure S6 IRC analysis of several typical pathways to low-lying isomers computed at the M06-2X/*aug-cc-p*VTZ level of theory.

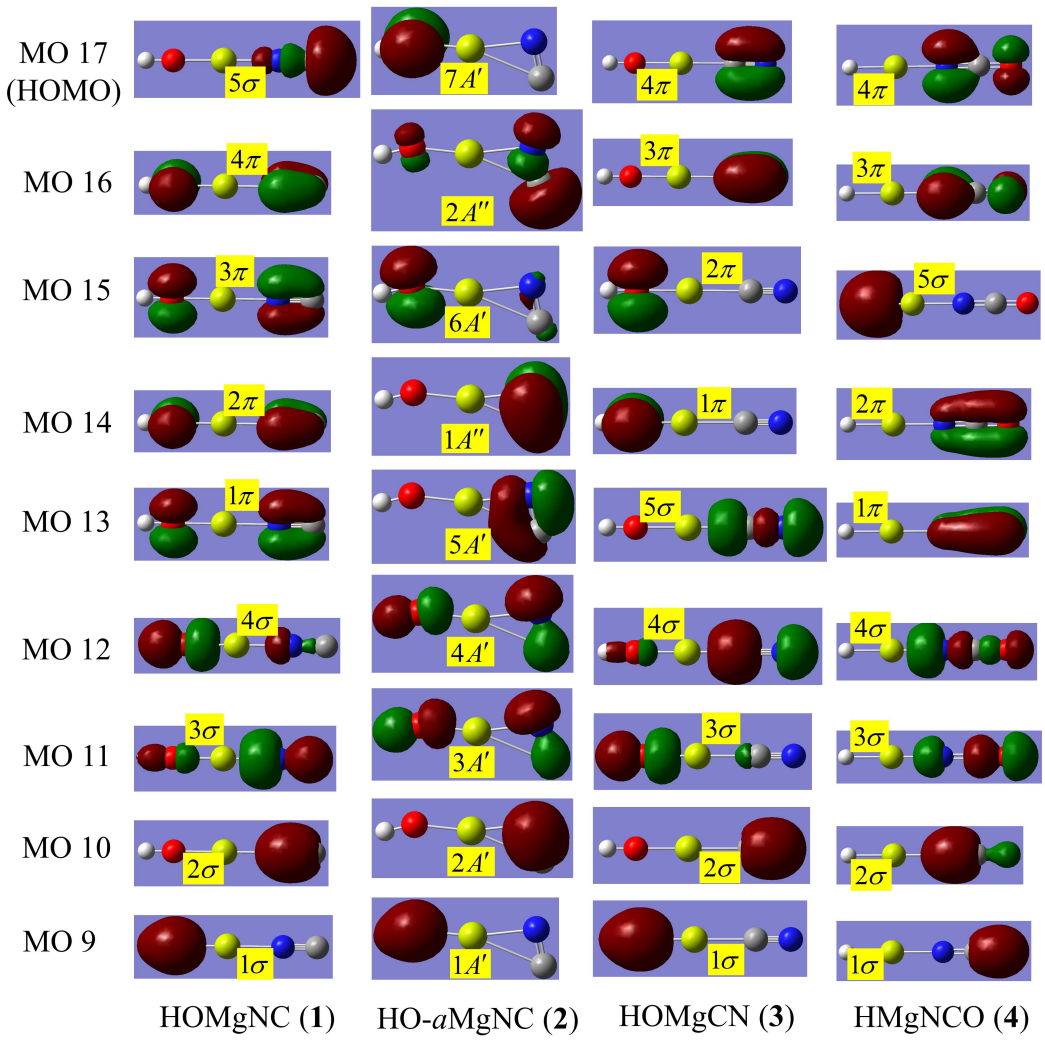
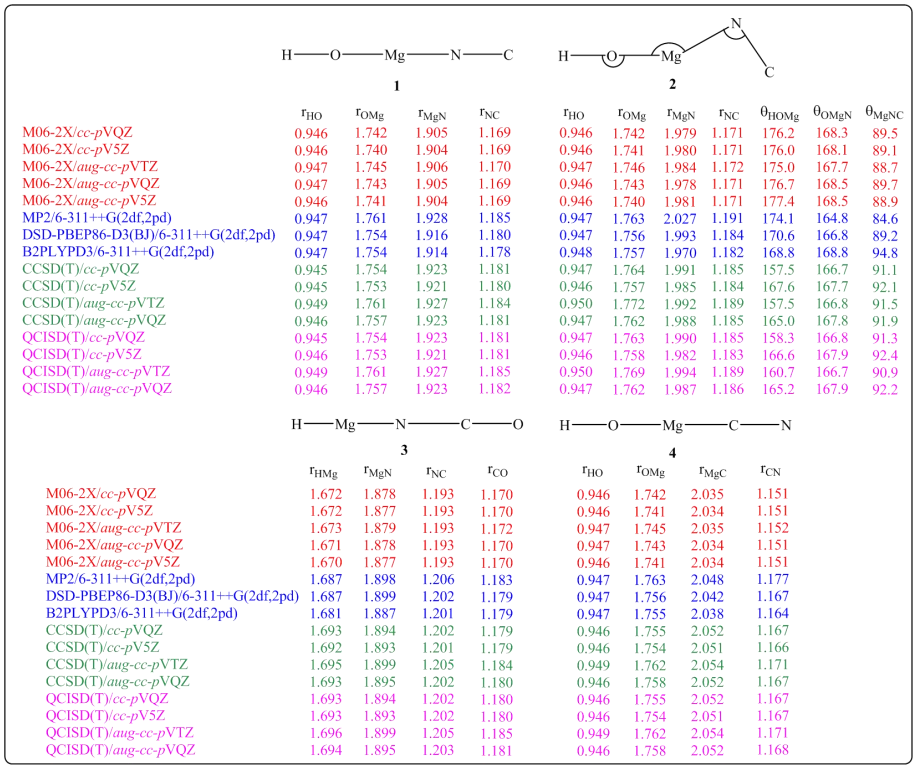


Figure S7 Valence molecule orbital pictures computed at the M06-2X/aug-cc-pVTZ level of theory.



	r_{HO}	r_{OMg}	r_{MgN}	r_{NC}	r_{HO}	r_{OMg}	r_{MgN}	r_{NC}	θ_{HOMg}	θ_{OMgN}	θ_{MgNC}
M06-2X/*cc-p*VQZ	0.946	1.742	1.905	1.169	0.946	1.742	1.979	1.171	176.2	168.3	89.5
M06-2X/*cc-p*V5Z	0.946	1.740	1.904	1.169	0.946	1.741	1.980	1.171	176.0	168.1	89.1
M06-2X/*aug-cc-p*VTZ	0.947	1.745	1.906	1.170	0.947	1.746	1.984	1.172	175.0	167.7	88.7
M06-2X/*aug-cc-p*VQZ	0.947	1.743	1.905	1.169	0.946	1.743	1.978	1.171	176.7	168.5	89.7
M06-2X/*aug-cc-p*V5Z	0.946	1.741	1.904	1.169	0.946	1.740	1.981	1.171	177.4	168.5	88.9
MP2/6-311++G(2df,2pd)	0.947	1.761	1.928	1.185	0.947	1.763	2.027	1.191	174.1	164.8	84.6
DSD-PBEP86-D3(BJ)/6-311++G(2df,2pd)	0.947	1.754	1.916	1.180	0.947	1.756	1.993	1.184	170.6	166.8	89.2
B2PLYPD3/6-311++G(2df,2pd)	0.947	1.754	1.914	1.178	0.948	1.757	1.970	1.182	168.8	168.8	94.8
CCSD(T)/*cc-p*VQZ	0.945	1.754	1.923	1.181	0.947	1.764	1.991	1.185	157.5	166.7	91.1
CCSD(T)/*cc-p*V5Z	0.945	1.753	1.921	1.180	0.946	1.757	1.985	1.184	167.6	167.7	92.1
CCSD(T)/*aug-cc-p*VTZ	0.949	1.761	1.927	1.184	0.950	1.772	1.992	1.189	157.5	166.8	91.5
CCSD(T)/*aug-cc-p*VQZ	0.946	1.757	1.923	1.181	0.947	1.762	1.988	1.185	165.0	167.8	91.9
QCISD(T)/*cc-p*VQZ	0.945	1.754	1.923	1.181	0.947	1.763	1.990	1.185	158.3	166.8	91.3
QCISD(T)/*cc-p*V5Z	0.946	1.753	1.921	1.181	0.946	1.758	1.982	1.183	166.6	167.9	92.4
QCISD(T)/*aug-cc-p*VTZ	0.949	1.761	1.927	1.185	0.950	1.769	1.994	1.189	160.7	166.7	90.9
QCISD(T)/*aug-cc-p*VQZ	0.946	1.757	1.923	1.182	0.947	1.762	1.987	1.186	165.2	167.9	92.2

	r_{HMg}	r_{MgN}	r_{NC}	r_{CO}	r_{HO}	r_{OMg}	r_{MgC}	r_{CN}
M06-2X/*cc-p*VQZ	1.672	1.878	1.193	1.170	0.946	1.742	2.035	1.151
M06-2X/*cc-p*V5Z	1.672	1.877	1.193	1.170	0.946	1.741	2.034	1.151
M06-2X/*aug-cc-p*VTZ	1.673	1.879	1.193	1.172	0.947	1.745	2.035	1.152
M06-2X/*aug-cc-p*VQZ	1.671	1.878	1.193	1.170	0.947	1.743	2.034	1.151
M06-2X/*aug-cc-p*V5Z	1.670	1.877	1.193	1.170	0.946	1.741	2.034	1.151
MP2/6-311++G(2df,2pd)	1.687	1.898	1.206	1.183	0.947	1.763	2.048	1.177
DSD-PBEP86-D3(BJ)/6-311++G(2df,2pd)	1.687	1.899	1.202	1.179	0.947	1.756	2.042	1.167
B2PLYPD3/6-311++G(2df,2pd)	1.681	1.887	1.201	1.179	0.947	1.755	2.038	1.164
CCSD(T)/*cc-p*VQZ	1.693	1.894	1.202	1.179	0.946	1.755	2.052	1.167
CCSD(T)/*cc-p*V5Z	1.692	1.893	1.201	1.179	0.946	1.754	2.051	1.166
CCSD(T)/*aug-cc-p*VTZ	1.695	1.899	1.205	1.184	0.949	1.762	2.054	1.171
CCSD(T)/*aug-cc-p*VQZ	1.693	1.895	1.202	1.180	0.946	1.758	2.052	1.167
QCISD(T)/*cc-p*VQZ	1.693	1.894	1.202	1.180	0.946	1.755	2.052	1.167
QCISD(T)/*cc-p*V5Z	1.693	1.893	1.202	1.180	0.946	1.754	2.051	1.167
QCISD(T)/*aug-cc-p*VTZ	1.696	1.899	1.205	1.185	0.949	1.762	2.054	1.171
QCISD(T)/*aug-cc-p*VQZ	1.694	1.895	1.203	1.181	0.946	1.758	2.052	1.168

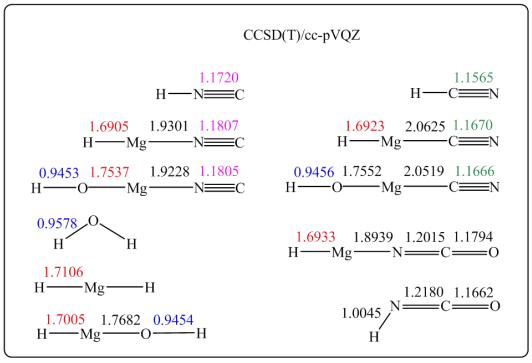


Figure S8 Geometry parameters of the isomers **1**, **2**, **3**, and **4** and several reference molecules optimized at various levels of theory.

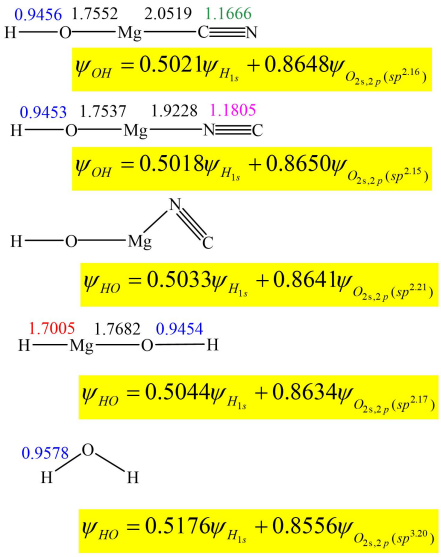


Figure S9 Character analysis of H-O hybrid orbit using the NBO technique computed at the CCSD(T)/*cc-p*VQZ level of theory

Table S1 Total electronic energies with ZPVE correction (E, in a.u.), ZPVE (in a.u.), enthalpies (H, in a.u., 298.15 K), and Gibbs free energies (G, in a.u., 298.15 K) of the [H,Mg,N,C,O] isomers and TSs in electronic singlet states computed at the M06-2X/*aug-cc-p*VTZ level of theory

Species	ZPVE	E	H	G
1	0.019205	-368.786360	-368.778674	-368.814327
2	0.018606	-368.784813	-368.777207	-368.814990
3	0.019640	-368.782379	-368.774867	-368.809925
4	0.018596	-368.772685	-368.766532	-368.798892
5	0.017821	-368.743063	-368.736642	-368.770143
6	0.021864	-368.725339	-368.718759	-368.756418
7	0.021834	-368.724917	-368.718259	-368.756418
8	0.023059	-368.708232	-368.703199	-368.734660
9	0.023180	-368.707250	-368.702585	-368.733397
10	0.022511	-368.688723	-368.682435	-368.718297
11	0.022275	-368.685699	-368.678910	-368.717734
12	0.021065	-368.665857	-368.659905	-368.693404
13	0.017889	-368.644687	-368.638485	-368.670672
14	0.016090	-368.640717	-368.634588	-368.668526
15	0.014236	-368.605048	-368.598800	-368.632646
16	0.021372	-368.596046	-368.589346	-368.626107
17	0.021314	-368.593062	-368.585994	-368.626403
Mg(^{1}S) + HONC (^{1}A′)	0.020962	-368.592314	-368.587727	-368.615661
Mg(^{1}S) + HOCN (^{1}A′)	0.021981	-368.684574	-368.680320	-368.707671
Mg(^{1}S) + HNCO (^{1}A′)	0.021484	-368.724294	-368.720110	-368.747175
TS1	0.019861	-368.647291	-368.641707	-368.674485
TS2	0.018825	-368.775580	-368.768828	-368.804461
TS3	0.016754	-368.672045	-368.666997	-368.698787
TS4	0.017438	-368.737312	-368.732200	-368.764046
TS5	0.015865	-368.665569	-368.660568	-368.691805
TS6	0.016305	-368.675551	-368.670391	-368.702366
TS7	0.020086	-368.666624	-368.661163	-368.693809
TS8	0.015256	-368.640449	-368.634475	-368.668834
TS9	0.017008	-368.643300	-368.637833	-368.670985
TS10	0.021149	-368.665515	-368.660146	-368.692663
TS11	0.018694	-368.639543	-368.634147	-368.666505
TS12	0.015818	-368.568943	-368.563734	-368.595773
TS13	0.018584	-368.784275	-368.777492	-368.813231
TS14	0.016482	-368.624507	-368.619282	-368.651306
TS15	0.016106	-368.643817	-368.637902	-368.673062
TS16	0.013788	-368.597744	-368.591799	-368.625214
TS17	0.013314	-368.598101	-368.592105	-368.625624
TS18	0.021933	-368.703285	-368.698114	-368.730295
TS19	0.021114	-368.590317	-368.584448	-368.618708

Table S2 Relative electronic energies with ZPVE correction (ΔE, in kcal mol^{-1}), relative enthalpies (ΔH, in kcal mol^{-1}, 298.15 K), and relative Gibbs free energies (ΔG, in kcal mol^{-1}, 298.15 K) of the [H,Mg,N,C,O] isomers and TSs in electronic singlet states computed at the M06-2X/*aug-cc-p*VTZ level of theory. These values were calculated with respective to the lowest-lying isomer **1**

Species	ΔE	ΔH	ΔG
1	0.0	0.0	0.0
2	1.0	0.9	-0.4
3	2.5	2.4	2.8
4	8.6	7.6	9.7
5	27.2	26.4	27.7
6	38.3	37.6	36.3
7	38.6	37.9	36.3
8	49.0	47.4	50.0
9	49.6	47.7	50.8
10	61.3	60.4	60.3
11	63.2	62.6	60.6
12	75.6	74.5	75.9
13	88.9	88.0	90.1
14	91.4	90.4	91.5
15	113.8	112.9	114.0
16	119.4	118.8	118.1
17	121.3	120.9	117.9
Mg(^{1}S) + HONC (^{1}A′)	121.8	119.8	124.7
Mg(^{1}S) + HOCN (^{1}A′)	63.9	61.7	66.9
Mg(^{1}S) + HNCO (^{1}A′)	38.9	36.7	42.1
TS1	87.3	85.9	87.8
TS2	6.8	6.2	6.2
TS3	71.7	70.1	72.5
TS4	30.8	29.2	31.6
TS5	75.8	74.1	76.9
TS6	69.5	67.9	70.3
TS7	75.1	73.7	75.6
TS8	91.6	90.5	91.3
TS9	89.8	88.4	89.9
TS10	75.8	74.4	76.3
TS11	92.1	90.7	92.8
TS12	136.4	134.9	137.1
TS13	1.3	0.7	0.7
TS14	101.6	100.0	102.3
TS15	89.4	88.3	88.6
TS16	118.4	117.3	118.7
TS17	118.1	117.1	118.4
TS18	52.1	50.6	52.7
TS19	123.0	121.9	122.8

Table S3 Total electronic energies with ZPVE correction (E, in a.u.), ZPVE (in a.u.), enthalpies (H, in a.u., 298.15 K), and Gibbs free energies (G, in a.u., 298.15 K) of the [H,Mg,N,C,O] isomers and TSs in electronic triplet states computed at the M06-2X/*aug-cc-p*VTZ level of theory

Species	ZPVE	E	H	G
1t	0.023141	-368.696003	-368.690726	-368.723839
2t	0.022434	-368.686903	-368.681375	-368.715322
3t	0.021926	-368.680393	-368.674925	-368.708670
4t	0.021773	-368.673782	-368.668233	-368.702134
5t	0.022442	-368.663970	-368.658414	-368.692251
6t	0.022791	-368.663642	-368.658042	-368.691969
7t	0.021701	-368.661829	-368.656412	-368.690145
8t	0.021616	-368.661426	-368.655624	-368.691137
9t	0.022541	-368.660585	-368.654664	-368.689325
10t	0.022026	-368.659765	-368.653792	-368.688883
11t	0.018325	-368.639294	-368.632372	-368.669407
12t	0.018962	-368.638124	-368.631347	-368.667844
13t	0.019078	-368.635618	-368.628906	-368.665883
14t	0.019014	-368.613725	-368.606792	-368.644572
15t	0.017649	-368.626406	-368.619146	-368.653807
TS1t	0.012886	-368.668019	-368.662442	-368.696240
TS2t	0.022136	-368.660038	-368.654816	-368.688108
TS3t	0.021681	-368.660795	-368.655957	-368.688773
TS4t	0.016793	-368.616516	-368.611111	-368.644536
TS5t	0.014546	-368.621863	-368.615833	-368.650786
TS6t	0.020384	-368.630272	-368.625008	-368.658459
TS7t	0.021415	-368.655270	-368.650008	-368.683363
TS8t	0.020717	-368.649997	-368.644239	-368.678908
TS9t	0.017858	-368.634127	-368.627800	-368.663669
TS10t	0.019027	-368.629021	-368.623303	-368.657896
TS11t	0.017721	-368.620677	-368.613947	-368.651629
TS12t	0.015161	-368.652919	-368.647157	-368.681226
TS13t	0.020467	-368.664212	-368.658727	-368.693106
TS14t	0.020610	-368.660870	-368.655854	-368.688483
TS15t	0.021455	-368.662023	-368.657323	-368.689485
TS16t	0.016483	-368.618784	-368.613105	-368.647547
TS17t	0.018580	-368.607218	-368.601164	-368.636145
TS18t	0.016991	-368.624275	-368.617477	-368.655375
$OH(^2\Pi)$ + MgNC ($^2\Sigma$)	0.015257	-368.617175	-368.608923	-368.658632
$HNC(^1\Sigma)$ + $MgO(^3\Pi)$	0.017456	-368.597878	-368.590727	-368.639311
$H(^2S)$ + MgNCO ($^2\Sigma$)	0.012272	-368.641760	-368.636611	-368.669428

Table S4 Relative electronic energies with ZPVE correction (ΔE, in kcal mol^{-1}), relative enthalpies (ΔH, in kcal mol^{-1}, 298.15 K), and relative Gibbs free energies (ΔG, in kcal mol^{-1}, 298.15 K) of the [H,Mg,N,C,O] isomers and TSs in electronic triplet states computed at the M06-2X/*aug-cc-p*VTZ level of theory. These values were calculated with respective to the lowest-lying isomer **1**

Species	ΔE	ΔH	ΔG
1t	56.4	55.1	56.8
2t	62.1	61.0	62.1
3t	66.2	65.0	66.3
4t	70.4	69.2	70.4
5t	76.5	75.4	76.6
6t	76.7	75.6	76.8
7t	77.9	76.6	77.9
8t	78.1	77.1	77.3
9t	78.6	77.7	78.4
10t	79.1	78.3	78.7
11t	92.0	91.7	90.9
12t	92.7	92.4	91.9
13t	94.3	93.9	93.2
14t	108.0	107.8	106.5
15t	100.1	99.1	100.7
TS1t	74.0	72.9	74.1
TS2t	79.0	77.6	79.2
TS3t	78.5	76.9	78.8
TS4t	106.3	105.1	106.5
TS5t	102.9	102.1	102.6
TS6t	97.7	96.3	97.8
TS7t	82.0	80.7	82.2
TS8t	85.3	84.3	85.0
TS9t	95.2	94.6	94.5
TS10t	98.4	97.4	98.2
TS11t	103.7	103.3	102.1
TS12t	83.4	82.4	83.5
TS13t	76.4	75.2	76.1
TS14t	78.5	77.0	79.0
TS15t	77.7	76.1	78.3
TS16t	104.9	103.8	104.7
TS17t	112.1	111.3	111.8
TS18t	101.4	101.1	99.7
OH($^2\Pi$) + MgNC ($^2\Sigma$)	105.9	106.4	97.7
HNC($^1\Sigma$) + MgO($^3\Pi$)	118.0	117.9	109.8
H(^{2}S) + MgNCO ($^2\Sigma$)	90.4	89.1	90.9

Table S5 Total electronic energies with ZPVE correction (E, in a.u.) of the isomers **1**, **2**, **3**, and **4** at various levels of theory

Level of theory	**1**	**2**	**3**	**4**
M06-2X/*aug-cc-p*VTZ	-368.786360	-368.784672	-368.782379	-368.772685
M06-2X/*aug-cc-p*VQZ	-368.796473	-368.794675	-368.792291	-368.782985
M06-2X/*aug-cc-p*V5Z	-368.802990	-368.801427	-368.798839	-368.788963
M06-2X/*cc-p*VQZ	-368.794511	-368.792918	-368.790431	-368.781539
M06-2X/*cc-p*V5Z	-368.802062	-368.800601	-368.798052	-368.788251
M06-2X/6-311++G(d,p)	-368.754801	-368.751874	-368.752524	-368.744328
M06-2X/6-311++G(2df,2pd)	-368.768230	-368.766690	-368.764968	-368.756776
M06-2X/6-311G(3df,3pd)	-368.769132	-368.768221	-368.765357	-368.756244
MP2/6-311++G(2df,2pd)	-368.082116	-368.081312	-368.085286	-368.069332
MP2/6-311G(3df,3pd)	-368.088368	-368.087865	-368.090886	-368.073860
DSD-PBEP86-D3(BJ)/6-311++G(2df,2pd)	-368.308405	-368.306378	-368.308706	-368.299975
DSD-PBEP86-D3(BJ)/6-311G(3df,3pd)	-368.311636	-368.309987	-368.311386	-368.301799
DSD-PBEP86-D3(BJ)/6-311++G(3df,3pd)	-368.314834	-368.312530	-368.315074	-368.305895
DSD-PBEP86-D3(BJ)/6-311+G(2df,2pd)	-368.308422	-368.306355	-368.308693	-368.299950
revDSD-PBEP86-D3(BJ)/6-311++G(2df,2pd)	-368.300440	-368.298315	-368.300738	-368.291583
revDSD-PBEP86-D3(BJ)/6-311G(3df,3pd)	-368.303748	-368.301967	-368.303505	-368.293462
B2PLYPD/6-311++G(d,p)	-368.588948	-368.586129	-368.590011	-368.581483
B2PLYPD/6-311++G(2df,2pd)	-368.628146	-368.625187	-368.627693	-368.619504
B2PLYPD/6-311G(3df,3pd)	-368.630120	-368.627483	-368.629046	-368.620028
B2PLYPD/6-311++G(3df,3pd)	-368.633319	-368.630076	-368.632826	-368.624335
CCSD(T)/*cc-p*VQZ	-368.182521	-368.180476	-368.181203	-368.166077
CCSD(T)/*cc-p*V5Z	-368.201243	-368.199266	-368.199788	-368.183738
CCSD(T)/*aug-cc-p*VTZ	-368.143341	-368.140944	-368.142054	-368.126199
CCSD(T)/*aug-cc-p*VQZ	-368.189231	-368.186742	-368.187657	-368.171621
QCISD(T)/*cc-p*VQZ	-368.183479	-368.181361	-368.182051	-368.167332
QCISD(T)/*aug-cc-p*VTZ	-368.144384	-368.142026	-368.142937	-368.127518
QCISD(T)/*aug-cc-p*VQZ	-368.190216	-368.187666	-368.188400	-368.172870

Table S6 Relative energies (in kcal mol^{-1}) of the isomers **1**, **2**, **3**, and **4** with ZPVE correction computed at various levels of theory

Level of theory	**1**	**2**	**3**	**4**
M06-2X/*aug-cc-p*VTZ	0.0	1.1	2.5	8.6
M06-2X/*aug-cc-p*VQZ	0.0	1.1	2.6	8.5
M06-2X/*aug-cc-p*V5Z	0.0	1.0	2.6	8.8
M06-2X/*cc-p*VQZ	0.0	1.0	2.6	8.1
M06-2X/*cc-p*V5Z	0.0	0.9	2.5	8.7
M06-2X/6-311++G(d,p)	0.0	1.8	1.4	6.6
M06-2X/6-311++G(2df,2pd)	0.0	1.0	2.1	7.2
M06-2X/6-311G(3df,3pd)	0.0	0.6	2.4	8.1
MP2/6-311++G(2df,2pd)	0.0	0.5	-2.0	8.0
MP2/6-311G(3df,3pd)	0.0	0.3	-1.6	9.1
DSD-PBEP86-D3(BJ)/6-311++G(2df,2pd)	0.0	1.3	-0.2	5.3
DSD-PBEP86-D3(BJ)/6-311G(3df,3pd)	0.0	1.0	0.2	6.2
DSD-PBEP86-D3(BJ)/6-311++G(3df,3pd)	0.0	1.5	-0.2	5.6
DSD-PBEP86-D3(BJ)/6-311+G(2df,2pd)	0.0	1.3	-0.2	5.3
revDSD-PBEP86-D3(BJ)/6-311++G(2df,2pd)	0.0	1.3	-0.2	5.6
revDSD-PBEP86-D3(BJ)/6-311G(3df,3pd)	0.0	1.1	0.2	6.5
B2PLYPD/6-311++G(d,p)	0.0	1.8	-0.7	4.7
B2PLYPD/6-311++G(2df,2pd)	0.0	1.9	0.3	5.4
B2PLYPD/6-311G(3df,3pd)	0.0	1.7	0.7	6.3
B2PLYPD/6-311++G(3df,3pd)	0.0	2.0	0.3	5.6
CCSD(T)/*cc-p*VQZ	0.0	1.3	0.8	10.3
CCSD(T)/*cc-p*V5Z	0.0	1.2	0.9	11.0
CCSD(T)/*aug-cc-p*VTZ	0.0	1.5	0.8	10.8
CCSD(T)/*aug-cc-p*VQZ	0.0	1.6	1.0	11.1
QCISD(T)/*cc-p*VQZ	0.0	1.3	0.9	10.1
QCISD(T)/*aug-cc-p*VTZ	0.0	1.5	0.9	10.6
QCISD(T)/*aug-cc-p*VQZ	0.0	1.6	1.1	10.9

Table S7 Imaginary frequency number at various levels of theory. When the optimization towards **2** leads to the linear structure **1**, the virgule symbol '/' is used

Computational levels	**1**	**2**	**3**	**4**
CCSD(T)/*cc-p*VDZ	0	0	0	0
CCSD(T)/*cc-p*VTZ	2i	0	2i	0
CCSD(T)/*cc-p*VQZ	0	0	0	0
CCSD(T)/*cc-p*V5Z	0	0	0	0
CCSD(T)/*aug-cc-p*VDZ	2i	/	2i	0
CCSD(T)/*aug-cc-p*VTZ	0	0	0	0
CCSD(T)/*aug-cc-p*VQZ	0	0	0	0
QCISD(T)/*cc-p*VDZ	0	0	0	0
QCISD(T)/*cc-p*VTZ	2i	0	2i	0
QCISD(T)/*cc-p*VQZ	0	0	0	0
QCISD(T)/*cc-p*V5Z	0	0	0	0
QCISD(T)/*aug-cc-p*VDZ	2i	/	2i	0
QCISD(T)/*aug-cc-p*VTZ	0	0	0	0
QCISD(T)/*aug-cc-p*VQZ	0	0	0	0
B3LYP/6-311G(d,p)	2i	/	2i	0
B3LYP/6-311G(2df,p)	2i	/	2i	0
B3LYP/6-311G(2df,2pd)	2i	/	2i	0
B3LYP/6-311++G(d,p)	0	/	0	0
B3LYP/6-311++G(3df,3pd)	0	/	0	0
B3LYP/6-311G(3df,3pd)	0	/	0	0
B3LYP/6-311+G(3df,3pd)	0	/	0	0
B3LYP/6-311++G(2df,2pd)	0	/	0	0
B3LYP/6-311+G(2df,p)	0	/	0	0
B3LYP/6-311+G(2df,2p)	0	/	0	0
B3LYP/6-311+G(2df,2pd)	0	/	0	0
B3LYP/6-311+G(2d,2p)	2i	/	0	0
B3LYP/6-311G(2d,2p)	2i	/	2i	0
B3LYP/6-311++G(2d,2p)	2i	/	0	0
B3LYP-D3(BJ)/6-311G(d,p)	2i	/	2i	0
B3LYP-D3(BJ)/6-311G(2df,p)	2i	/	2i	0
B3LYP-D3(BJ)/6-311G(2df,2pd)	2i	/	2i	0
B3LYP-D3(BJ)/6-311++G(d,p)	0	/	0	0
B3LYP-D3(BJ)/6-311++G(3df,3pd)	0	/	0	0
B3LYP-D3(BJ)/6-311G(3df,3pd)	0	/	0	0
B3LYP-D3(BJ)/6-311+G(3df,3pd)	0	/	0	0
B3LYP-D3(BJ)/6-311++G(2df,2pd)	0	/	0	0
B3LYP-D3(BJ)/6-311+G(2df,p)	0	/	0	0
B3LYP-D3(BJ)/6-311+G(2df,2p)	0	/	0	0
B3LYP-D3(BJ)/6-311+G(2df,2pd)	0	/	0	0
B3LYP-D3(BJ)/6-311+G(2d,2p)	2i	/	0	0
B3LYP-D3(BJ)/6-311G(2d,2p)	2i	/	2i	0
B3LYP-D3(BJ)/6-311++G(2d,2p)	2i	/	0	0
M06-2X/ *cc-p*VDZ	2i	0	2i	0
M06-2X/*cc-p*VTZ	2i	1i	0	0
M06-2X/*cc-p*VQZ	0	0	0	0
M06-2X/*cc-p*V5Z	0	0	0	0
M06-2X/*aug-cc-p*VDZ	2i	0	2i	0
M06-2X/*aug-cc-p*VTZ	0	0	0	0
M06-2X/*aug-cc-p*VQZ	0	0	0	0
M06-2X/*aug-cc-p*V5Z	0	0	0	0
MP2/6-311G(d,p)	2i	1i	2i	0
MP2/6-311++G(d,p)	2i	1i	2i	0
MP2/6-311G(2d,2p)	2i	0	2i	0

Table S7 (Continued)

Computational levels	**1**	**2**	**3**	**4**
MP2/6-311+G(2d,2p)	0	0	0	0
MP2/6-311++G(2d,2p)	0	0	0	0
MP2/6-311G(2df,2pd)	0	0	0	0
MP2/6-311+G(2df,2pd)	0	0	0	0
MP2/6-311++G(2df,2pd)	0	0	0	0
MP2/6-311G(3df,3pd)	0	0	0	0
MP2/6-311+G(3df,3pd)	0	0	0	0
MP2/6-311++G(3df,3pd)	0	0	0	0
ωB97XD/6-311++G(3df,3pd)	0	/	0	0
ωB97XD/6-311++G(2df,2pd)	0	/	0	0
ωB97XD/*aug-cc-p*VTZ	0	/	0	0
ωB97XD/*aug-cc-p*VQZ	0	/	0	0
ωB97XD/6-311G(3df,3pd)	0	/	0	0
ωB97XD/6-311G(2df,2pd)	0	/	0	0
ωB97XD/6-311G(2d,2p)	0	/	0	0
ωB97XD/6-311++G(2d,2p)	0	/	0	0
ωB97XD/6-311++G(d,p)	0	/	0	0
ωB97XD/6-311G(d,p)	0	/	0	0
DSD-PBEP86-D3(BJ)/6-311G(d,p)	2i	0	2i	0
DSD-PBEP86-D3(BJ)/6-311G(2df,p)	2i	0	2i	0
DSD-PBEP86-D3(BJ)/6-311++G(d,p)	0	1i	0	0
DSD-PBEP86-D3(BJ)/6-311G(2df,2pd)	2i	0	0	0
DSD-PBEP86-D3(BJ)/6-311++G(2d,2p)	0	0	0	0
DSD-PBEP86-D3(BJ)/6-311++G(2df,2pd)	0	0	0	0
DSD-PBEP86-D3(BJ)/6-311++G(3df,3pd)	0	0	0	0
DSD-PBEP86-D3(BJ)/6-311G(3df,3pd)	0	0	0	0
DSD-PBEP86-D3(BJ)/6-311+G(3df,3pd)	0	0	0	0
DSD-PBEP86-D3(BJ)/6-311+G(2df,p)	0	0	0	0
DSD-PBEP86-D3(BJ)/6-311+G(2df,2p)	0	0	0	0
DSD-PBEP86-D3(BJ)/6-311+G(2df,2pd)	0	0	0	0
revDSD-PBEP86-D3(BJ)/6-311G(d,p)	2i	0	2i	0
revDSD-PBEP86-D3(BJ)/6-311G(2df,p)	2i	0	2i	0
revDSD-PBEP86-D3(BJ)/6-311++G(d,p)	0	1i	0	0
revDSD-PBEP86-D3(BJ)/6-311G(2df,2pd)	2i	0	0	0
revDSD-PBEP86-D3(BJ)/6-311++G(2d,2p)	0	0	0	0
revDSD-PBEP86-D3(BJ)/6-311++G(2df,2pd)	0	0	0	0
revDSD-PBEP86-D3(BJ)/6-311++G(3df,3pd)	0	0	0	0
revDSD-PBEP86-D3(BJ)/6-311G(3df,3pd)	0	0	0	0
revDSD-PBEP86-D3(BJ)/6-311+G(3df,3pd)	0	0	0	0
revDSD-PBEP86-D3(BJ)/6-311+G(2df,p)	0	0	0	0
revDSD-PBEP86-D3(BJ)/6-311+G(2df,2p)	0	0	0	0
revDSD-PBEP86-D3(BJ)/6-311+G(2df,2pd)	0	0	0	0
B2PLYPD3/6-311G(d,p)	2i	0	2i	0
B2PLYPD/6-311G(2df,p)	2i	0	2i	0
B2PLYPD/6-311G(2df,2pd)	2i	0	2i	0
B2PLYPD/6-311G(3df,3pd)	0	0	0	0
B2PLYPD/6-311++G(d,p)	0	0	0	0
B2PLYPD/6-311++G(2d,2p)	0	0	0	0
B2PLYPD/6-311++G(2df,2pd)	0	0	0	0
B2PLYPD/6-311++G(3df,3pd)	0	0	0	0
B2PLYPD/6-311+G(3df,3pd)	0	0	0	0
B2PLYPD/6-311+G(2df,p)	0	0	0	0
B2PLYPD/6-311+G(2df,2p)	0	0	0	0
B2PLYPD/6-311+G(2df,2pd)	0	0	0	0

Table S8 Basin charge, AIM charge, natural population charge (NPC), and Mulliken charge of the isomers **1**, **2**, **3**, **4**, and reference molecules computed at the CCSD(T)/*cc-p*VQZ level of theory

Species	Atom	Basin charge	AIM charge	NPC	Mulliken charge
HOMgNC (**1**) ($^1\Sigma$)	H	0.343	0.657	0.49	0.22
	O	9.561	-1.563	-1.44	-0.71
	Mg	10.183	1.815	1.90	1.04
	N	9.023	-2.025	-1.23	-0.51
	C	4.882	1.117	0.28	-0.04
HOMgCN (**3**) ($^1\Sigma$)	H	0.339	0.660	0.49	0.22
	O	9.565	-1.567	-1.44	-0.70
	Mg	10.208	1.789	1.83	0.95
	C	5.397	0.602	-0.47	-0.25
	N	8.483	-1.485	-0.42	-0.22
HMgNCO (**4**) ($^1\Sigma$)	H	1.789	-0.790	-0.74	-0.24
	Mg	10.298	1.699	1.67	0.79
	N	8.956	-1.958	-1.26	-0.70
	C	3.544	2.456	0.99	0.60
	O	9.406	-1.408	-0.66	-0.44
HOMgNC (**2**) (^{1}A)	H	0.346	0.654	0.49	0.22
	O	9.557	-1.559	-1.43	-0.70
	Mg	10.198	1.800	1.86	0.96
	N	8.901	-1.903	-0.97	-0.37
	C	4.991	1.008	0.05	-0.11
NCMgCN ($^1\Sigma$)	N	8.459	-1.462	-0.39	-0.20
	C	5.413	0.585	-0.47	-0.25
	Mg	10.244	1.752	1.72	0.90
	C	5.413	0.585	-0.47	-0.25
	N	8.459	-1.462	-0.39	-0.20
CNMgNC ($^1\Sigma$)	C	4.864	1.135	0.31	-0.03
	N	9.037	-2.039	-1.24	-0.48
	Mg	10.188	1.809	1.87	1.02
	N	9.037	-2.039	-1.24	-0.50
	C	4.864	1.135	0.31	-0.01
HMgNC ($^1\Sigma$)	H	1.786	-0.787	-0.72	-0.23
	Mg	10.299	1.699	1.65	0.80
	N	9.023	-2.025	-1.21	-0.52
	C	4.887	1.112	0.28	-0.04
HMgCN ($^1\Sigma$)	H	1.787	-0.787	-0.71	-0.23
	Mg	10.322	1.676	1.57	0.77
	C	5.400	0.599	-0.44	-0.32
	N	8.486	-1.488	-0.42	-0.21
HMgOH ($^1\Sigma$)	H	1.799	-0.799	-0.76	-0.26
	Mg	10.287	1.712	1.71	0.77
	O	9.559	-1.560	-1.43	-0.71
	H	0.354	0.646	0.49	0.21
HMgH ($^1\Sigma$)	H	1.811	-0.811	-0.73	-0.28
	Mg	10.378	1.621	1.45	0.56
	H	1.811	-0.811	-0.73	-0.28
HMg ($^2\Sigma$)	H	1.790	-0.790	-0.29	-0.29
	Mg	11.210	0.790	0.79	0.29
MgCN ($^2\Sigma$)	Mg	11.096	0.902	0.94	0.57
	C	5.392	0.606	-0.50	-0.34
	N	8.506	-1.508	-0.44	-0.23
MgNC ($^2\Sigma$)	Mg	11.068	0.930	1.00	0.55
	N	9.027	-2.028	-1.26	-0.48
	C	4.900	1.099	0.26	-0.07

Table S8 (Continued)

Species	Atom	Basin charge	AIM charge	NPC	Mulliken charge
MgOH ($^2\Sigma$)	Mg	11.064	0.935	0.97	0.49
	O	9.574	-1.575	-0.72	-0.68
	H	0.360	0.640	0.25	0.19
CN	C	4.779	1.219	0.45	0.17
	N	8.215	-1.219	-0.45	-0.17
HCN ($^1\Sigma$)	H	0.787	0.212	0.23	0.16
	C	4.801	1.195	0.11	0.03
	N	8.403	-1.408	-0.34	-0.19
HNC ($^1\Sigma$)	H	0.402	0.598	0.46	0.23
	N	8.780	-1.784	-0.83	-0.31
	C	4.812	1.186	0.37	0.08

Table S9 ELF values at BCPs for **1**, **2**, **3**, and **4** computed at the CCSD(T)/*aug-cc-p*VTZ level of theory

Species	Bond	ELF
1	H-O	0.984
	O-Mg	0.054
	Mg-N	0.065
	N-C	0.535
2	H-O	0.983
	O-Mg	0.056
	Mg-N	0.060
	N-C	0.547
3	H-O	0.984
	O-Mg	0.054
	Mg-C	0.086
	C-N	0.477
4	H-Mg	0.118
	Mg-N	0.062
	N-C	0.624
	C-O	0.488

Table S10 Local topological properties (in a.u.) of the electronic charge density distribution at BCPs for **1**, **2**, **3**, and **4** computed at the CCSD(T)/*aug-cc-p*VTZ level of theory

Species	Bond	$\rho(r)$	$\nabla^2\rho(r)$	$V(r)$	$G(r)$	$\lvert V(r)\rvert/G(r)$	$H(r)$
HOMgNC (**1**)	H-O	0.374	-2.892	-0.866	0.072	12.028	-0.795
	O-Mg	0.081	0.749	-0.178	0.183	0.973	0.004
	Mg-N	0.064	0.455	-0.111	0.113	0.982	0.001
	N-C	0.467	-0.523	-1.635	0.752	2.174	-0.883
HO-*a*MgNC (**2**)	H-O	0.374	-2.864	-0.862	0.073	11.808	-0.789
	O-Mg	0.081	0.726	-0.174	0.178	0.978	0.004
	Mg-N	0.053	0.342	-0.083	0.084	0.988	0.001
	N-C	0.473	-0.600	-1.649	0.750	2.199	-0.900
HOMgCN (**3**)	H-O	0.374	-2.891	-0.866	0.071	12.197	-0.794
	O-Mg	0.081	0.747	-0.178	0.182	0.978	0.004
	Mg-C	0.057	0.306	-0.082	0.079	1.038	-0.003
	C-N	0.483	-0.115	-1.815	0.893	2.032	-0.922
HMgNCO (**4**)	H-Mg	0.056	0.232	-0.071	0.064	1.109	-0.006
	Mg-N	0.066	0.484	-0.118	0.119	0.992	0.002
	N-C	0.447	-0.916	-1.395	0.583	2.393	-0.812
	C-O	0.451	-0.192	-1.605	0.779	2.060	-0.827

ρ(r), electronic charge density; $\nabla^2\rho(r)$, Laplacian function of electronic density, $\lvert V(r)\rvert/G(r)$, relationship between the potential energy density $V(r)$ and the Lagrangian form of kinetic energy density $G(r)$, define as energies density of the unit of electrons; and $H(r)$, total energy density, define as $V(r) + G(r)$.

Table S11 Cartesian coordinates of all located stationary points optimized at the M06-2X/*aug-cc-p*VTZ level of theory

Species	Geometries	Species	Geometries
1	H 0.00000 0.00000 3.13731 O 0.00000 0.00000 2.19016 Mg 0.00000 0.00000 0.44545 N 0.00000 0.00000 –1.46046 C 0.00000 0.00000 –2.63011	**2**	H –0.44534 2.94917 0.00000 O –0.29994 2.01329 0.00000 Mg 0.00000 0.29444 0.00000 N 0.72755 –1.55403 0.00000 C –0.37467 –1.95176 0.00000
3	H 0.00000 0.00000 3.21785 O 0.00000 0.00000 2.27056 Mg 0.00000 0.00000 0.52532 C 0.00000 0.00000 –1.50932 N 0.00000 0.00000 –2.66147	**4**	H 0.00000 0.00000 3.55132 Mg 0.00000 0.00000 1.87885 N 0.00000 0.00000 –0.00059 C 0.00000 0.00000 –1.19401 O 0.00000 0.00000 –2.36616
5	H 0.00000 0.00000 3.44803 Mg 0.00000 0.00000 1.78326 O 0.00000 0.00000 –0.01925 C 0.00000 0.00000 –1.27754 N 0.00000 0.00000 –2.43255	**6**	Mg 2.39836 –0.01698 0.00000 H –0.72705 –1.82295 –0.00003 C –1.29158 0.05319 –0.00001 O –1.25338 1.21223 0.00000 N –1.46811 –1.14147 0.00001
7	Mg –2.42077 0.03949 0.00138 N 1.28509 1.13816 –0.01591 C 1.33704 –0.06809 0.00143 O 1.24481 –1.22354 0.00103 H 2.07286 1.75584 0.07791	**8**	H 1.99021 0.91706 –0.00000 N 1.11450 0.42176 –0.00000 C 0.00000 1.08421 –0.00000 O –1.11206 0.51309 –0.00000 Mg –0.07460 –1.20661 0.00000
9	Mg –0.09336 –1.14303 0.00000 N –1.17828 0.50441 0.00000 C 0.00000 0.98686 0.00000 H 0.16887 2.07246 0.00000 O 1.14992 0.27399 0.00000	**10**	Mg –2.19781 0.02233 –0.00000 H 0.35275 –1.47518 0.00001 O 1.26285 –1.12537 0.00000 C 1.22787 0.16642 –0.00001 N 1.22156 1.31595 0.00000
11	Mg –2.70493 0.23781 0.00914 O 2.27230 0.64710 –0.05399 H 3.03747 0.36547 0.46457 C 1.33439 –0.24309 –0.01281 N 0.46242 –0.99106 –0.00936	**12**	Mg –1.22995 –0.16572 0.00103 H 1.39319 –1.58968 0.02205 O 0.64685 –0.97863 –0.00504 C 1.06961 0.39661 0.00186 N 0.25340 1.28967 –0.00075
13	H 0.00000 0.00000 3.66357 Mg 0.00000 0.00000 1.99150 C 0.00000 0.00000 –0.02309 N 0.00000 0.00000 –1.18857 O 0.00000 0.00000 –2.38789	**14**	H –0.92945 2.72456 –0.00000 Mg –0.13908 1.25788 –0.00000 O 1.08056 –0.20997 0.00000 N 0.00000 –0.96666 0.00000 C –1.00767 –1.56214 –0.00000
15	H –2.88451 –0.25579 0.29296 Mg –1.24367 –0.05597 0.05090 N 0.69268 –0.74061 –0.27768 C 1.54719 –0.12120 0.37899 O 0.45959 0.85486 –0.15424	**16**	Mg 2.24877 0.05587 –0.00002 H –0.27338 –1.34327 0.00079 O –1.22342 –1.11518 –0.00009 C –1.34477 1.36307 0.00003 N –1.26513 0.20227 0.00000
17	H 2.67614 –0.91438 –0.00392 O 1.70865 –0.93546 0.00070 N 1.31785 0.32639 –0.00032 C 0.81728 1.37769 0.00027 Mg –2.53949 –0.17941 –0.00009	**1t**	H 1.96689 0.99844 0.00000 N 1.13017 0.43705 0.00000 C 0.00000 1.08713 0.00000 O –1.11941 0.54542 0.00000 Mg –0.07690 –1.24532 0.00000
2t	H –0.31251 1.74691 –0.00002 N 0.07535 0.80360 0.00000 C –0.80144 –0.17718 0.00003 O –1.98228 –0.33984 –0.00002 Mg 1.70433 –0.29920 –0.00001	**3t**	Mg 1.31929 0.11639 0.04818 N –0.68283 1.11402 –0.09917 C –1.11499 –0.07713 0.08766 H –2.13927 –0.29030 0.41053 O –0.27781 –1.05522 –0.10256
4t	H 0.94471 2.41771 0.00000 N 0.01211 1.99420 0.00000 C 0.00000 0.75719 0.00000 O 0.79092 –0.25641 0.00000 Mg –0.61307 –1.57241 0.00000	**5t**	H –2.37124 0.45113 0.00000 O –1.87767 –0.38583 0.00000 C –0.56867 –0.10521 –0.00000 N 0.07863 0.94088 0.00000 Mg 1.68785 –0.27662 0.00000
6t	Mg –0.45741 –1.64263 0.00000 H –0.93827 2.22207 0.00000 O –0.02279 1.92901 0.00000 C 0.00000 0.58039 0.00000 N 0.94421 –0.20357 0.00000	**7t**	H –0.95110 –1.11779 0.94748 N –1.19036 –0.82435 –0.00949 C –0.89977 0.40030 –0.26536 Mg 1.21464 –0.40447 –0.04301 O 0.01332 1.16751 0.15341

Table S11 (Continued)

Species	Geometries	Species	Geometries
8t	Mg –1.98018 –0.15137 –0.06298 N –0.11363 0.30761 0.24035 C 1.18023 0.38675 –0.06986 H 1.45884 1.41792 –0.37791 O 2.00218 –0.50940 –0.01620	**9t**	Mg –2.06273 –0.03761 –0.00010 H 2.85761 0.38449 0.00012 O 2.14614 –0.26175 0.00012 C 0.96997 0.41465 0.00003 N –0.15625 –0.04672 –0.00001
10t	H 2.35902 –0.42499 0.00000 O 1.81847 –1.23441 0.00000 C 0.52520 –0.88077 0.00000 N 0.00000 0.22496 0.00000 Mg –1.67150 1.16751 0.00000	**11t**	H 0.00021 1.72592 0.54624 O 0.62019 1.31683 –0.08428 Mg 1.08220 –0.73036 0.02853 N –0.90788 –0.53065 –0.05114 C –1.93216 0.03636 0.02393
12t	H –0.06758 1.71547 0.41856 O 0.57370 1.17842 –0.06558 Mg 1.27751 –0.64697 0.02527 C –0.90909 –0.337590 –0.06731 N –2.05679 –0.19338 0.02954	**13t**	H 0.31679 –2.27207 0.00000 C –0.46434 –1.54181 0.00000 N –1.27111 –0.72991 0.00000 Mg 0.00000 1.33951 0.00000 O 1.42088 0.06977 0.00000
14t	H –3.03452 0.48126 0.00049 N –2.13595 0.04266 0.00012 C –1.07339 –0.40398 –0.00034 O 1.05347 1.20431 –0.00004 Mg 1.33323 –0.66588 0.00009	**15t**	Mg –2.55987 0.00321 0.00017 H 2.64024 0.00051 0.00026 O 3.62276 0.00333 –0.00016 C 0.55850 –0.00559 0.00120 N –0.60784 –0.00458 –0.00118
TS1	Mg –1.38708 –0.45542 –0.00004 O –0.19201 1.03176 0.00011 H 0.37489 1.81972 –0.00059 C 0.74209 –0.30229 0.00012 N 1.90766 –0.39929 –0.00006	**TS2**	Mg –0.40041 –0.13277 0.00000 O –2.13034 0.11036 0.00000 H –3.02596 0.41951 –0.00000 N 2.19833 0.47487 0.00000 C 1.58087 –0.50553 –0.00000
TS3	Mg –0.28646 –1.41313 –0.00000 H 1.41749 –0.40724 –0.00000 O 1.23222 0.92492 –0.00000 C –0.00000 0.96856 0.00000 N –1.11967 0.59343 0.00000	**TS4**	Mg –1.22884 –0.26667 0.00001 H –2.69199 –1.05971 –0.00003 O 0.12441 1.12803 –0.00000 C 0.95580 0.17985 –0.00000 N 1.52971 –0.83481 –0.00000
TS5	Mg –2.05083 0.00408 –0.01569 N –0.04112 –0.19254 0.03661 C 1.17038 –0.08592 0.00668 O 2.32267 0.07961 –0.02059 H –0.70583 1.17744 0.05662	**TS6**	Mg 1.35403 –0.34839 0.00000 H –0.08499 –1.51487 0.00000 C –0.94964 0.31091 0.00000 O –0.04923 1.15270 0.00000 N –1.43881 –0.77022 0.00000
TS7	Mg –1.18769 0.03146 0.00000 H 1.10894 1.78200 0.00006 O 0.46123 1.06822 –0.00001 C 1.13153 –0.30959 0.00001 N 0.38061 –1.26396 –0.00000	**TS8**	Mg 1.96844 –0.08942 –0.06514 O 0.00754 0.05263 0.18936 C –1.26205 –0.02420 0.03745 N –2.40467 –0.06161 –0.11434 H 0.72343 1.22853 –0.15751
TS9	Mg –1.68229 –0.30014 –0.00000 N –0.00000 1.00261 –0.00000 C 1.01182 0.24677 0.00000 O 1.58775 –0.79247 0.00000 H 1.41457 1.44255 –0.00000	**TS10**	Mg –1.30088 –0.28345 0.00000 N 0.13056 1.29191 0.00000 C 1.01139 0.47721 0.00000 O 0.86435 –0.89393 –0.00000 H 1.71362 –1.35385 0.00000
TS11	Mg 0.00000 –1.03382 –0.00000 H 0.63718 1.53043 0.00000 O 1.44596 –0.02063 –0.00000 C –0.41735 1.20118 0.00000 N –1.38583 0.54762 0.00000	**TS12**	Mg 1.42428 –0.22508 –0.00000 H 0.09046 –1.50646 –0.00000 O –1.22194 –0.82765 –0.00000 C –0.22217 1.36536 0.00000 N –0.86760 0.37665 0.00000
TS13	H 0.99699 2.85630 0.00000 O 0.56381 2.01383 0.00000 Mg 0.00000 0.36142 0.00000 N –0.78857 –1.39267 0.00000 C 0.00209 –2.25922 0.00000	**TS14**	Mg 1.26771 –0.15498 0.00003 N –0.83546 0.27596 –0.00001 C –0.30042 1.32913 –0.00001 H 2.70544 –0.99276 –0.00017 O –1.28340 –0.88176 0.00000
TS15	H 1.92791 –0.68132 –0.00078 N 0.70364 –1.08057 0.00011 C 0.96710 0.16646 0.00006 O 0.28049 1.20453 0.00002 Mg –1.24165 –0.19914 –0.00004	**TS16**	H 2.91288 –0.60705 0.00002 Mg 1.31272 –0.11988 –0.00000 O –0.27860 0.92456 –0.00000 N –0.72029 –0.53861 –0.00000 C –1.89912 –0.26343 0.00001

Table S11 (Continued)

Species	Geometries	Species	Geometries
TS17	H –2.84844 –0.36749 0.23969 Mg –1.21660 –0.06299 0.03301 N 0.76662 –0.89261 –0.19650 C 1.45797 –0.03968 0.30585 O 0.41669 0.95122 –0.13692	**TS18**	H 1.99117 0.93251 0.00000 N 1.09518 0.47432 0.00000 C 0.00000 1.08057 0.00000 O –1.15848 0.82878 0.00000 Mg –0.03246 –1.44720 0.00000
TS19	H 1.70012 1.95081 0.00000 O 1.33521 1.05624 0.00000 N 0.00000 1.21258 –0.00000 C –1.04339 0.65219 –0.00000 Mg –0.51012 –1.90017 0.00000	**TS1t**	H –2.43300 0.16931 0.00000 O –2.04963 –0.72512 0.00000 C –0.71331 –0.61184 0.00000 N 0.00000 0.38826 0.00000 Mg 1.92582 0.54874 0.00000
TS2t	Mg 1.93349 0.45696 0.00000 H –2.34427 –1.46762 0.00000 O –2.07107 –0.54600 0.00000 C –0.71485 –0.50926 0.00000 N 0.00000 0.48680 0.00000	**TS3t**	Mg 1.74438 –0.24785 0.06950 N 0.07161 0.75887 –0.27233 C –1.13374 0.37937 0.16057 H –1.68609 1.15016 0.73041 O –1.61817 –0.72054 –0.07768
TS4t	Mg –1.24099 –0.34141 0.03956 N 0.98391 –0.97085 –0.14155 C 0.94582 0.28985 0.05973 H 1.80361 –0.37089 0.69900 O 0.06576 1.19059 –0.06766	**TS5t**	H –0.25198 1.46798 –0.00081 O 0.95333 1.10261 0.00032 Mg 0.86171 –0.87117 –0.00015 N –1.51684 –0.49808 0.00042 C –1.18288 0.60861 –0.00048
TS6t	H 1.25549 –1.56656 0.00043 O 0.38336 –1.14474 –0.00003 C 0.53640 0.28006 –0.00026 N 1.62964 0.83956 0.00012 Mg –1.57902 0.26393 0.00005	**TS7t**	H 2.29191 –0.30808 0.77901 O 1.90577 –0.302295 –0.10497 C 0.56672 –0.05764 –0.00762 N –0.10399 0.96598 0.00182 Mg –1.68421 –0.30747 0.00781
TS8t	Mg 2.05542 0.00483 –0.00004 H –2.53148 –0.47319 0.67722 O –2.20238 –0.05663 –0.12866 C –0.91732 0.38374 0.09468 N 0.14135 –0.20489 –0.03080	**TS9t**	H 1.40094 1.37885 0.56377 O 1.52695 0.70486 –0.12759 Mg 0.35104 –1.03985 0.02970 C –1.95820 0.21706 –0.11182 N –0.86853 0.59401 0.11022
TS10t	Mg –1.29578 –0.35549 –0.00005 N 0.92740 –0.97774 0.00012 C 1.39809 0.08443 –0.00014 H 2.11040 0.88266 –0.00012 O –0.18017 1.21510 0.00008	**TS11t**	Mg 2.08591 –0.32360 0.00001 H –3.04983 0.16728 0.00107 O –2.43383 –0.57939 –0.00009 C –0.80240 0.79825 –0.00018 N 0.32914 0.50878 0.00009
TS12t	H –0.49175 1.31130 –0.00153 Mg –2.02918 –0.07964 –0.00102 N –0.07013 0.06845 0.00283 C 1.14045 –0.09515 0.00142 O 2.31126 –0.03298 –0.00183	**TS13t**	H 0.06802 1.64135 –0.29349 N 0.07519 0.72907 0.15827 C –0.96119 –0.04236 –0.33018 O –2.00263 –0.35568 0.13360 Mg 1.76616 –0.30377 0.00816
TS14t	H –0.77259 –1.42658 0.90596 N –0.76569 –1.06605 –0.04603 C –1.01332 0.21653 –0.19736 Mg 1.23089 –0.16510 –0.02981 O –0.31980 1.19638 0.11977	**TS15t**	H –1.07368 –1.08910 0.92083 N –1.33879 –0.73660 –0.00913 C –0.89583 0.42847 –0.26865 Mg 1.25823 –0.43524 –0.04345 O 0.09018 1.11217 0.15954
TS16t	Mg –1.95309 –0.19227 –0.05158 N –0.11779 0.36223 0.25678 C 1.12791 0.24319 –0.11630 H 0.39506 1.28947 –0.46899 O 2.13738 –0.37212 –0.00146	**TS17t**	H 2.90227 0.23024 0.00012 N 2.00242 –0.20319 –0.00004 C 0.85393 –0.38419 0.00003 O –0.45327 1.09985 –0.00000 Mg –1.53472 –0.44180 –0.00000
TS18t	Mg –1.87407 0.62303 –0.00013 H 2.41300 –0.20820 –0.00036 O 2.58279 0.75420 0.00008 C 0.52646 –1.28541 –0.00047 N –0.53503 –0.79847 0.00058		