Supporting Information: The Mechanism of Carbon Dioxide Adsorption in an Alkylamine-Functionalized Metal-Organic Framework

Nora Planas,[a]‡ Allison L. Dzubak,[a]‡ Roberta Poloni,[b,d] Li-Chiang Lin,[b] Alison McManus,[a] Thomas M. McDonald,[c,d] Jeffrey B. Neaton,[e] Jeffrey R. Long,[c,d] Berend Smit,[b,c,d*] Laura Gagliardi [a*]

[a] Department of Chemistry, Supercomputing Institute, and Chemical Theory Center, University of Minnesota Minneapolis, Minnesota, 55455, USA.

[b] Department of Chemical and Biomolecular Engineering, University of California, Berkeley, CA 94720, USA.

[c] Department of Chemistry, University of California, Berkeley, CA 94720, USA.

[d]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA.

[e]Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA.

‡These two authors equally contributed to the paper
*: gagliard@umn.edu, Berend-Smit@berkeley.edu;

==========

Contents of Supporting Information:

==========

1. Detailed acknowledgments

A.L.D. was supported by the US Department of Energy under contracts DE-FY12-SC0006860 (A.L.D.)

N.P., L.G., J.R.L., and. J.B.N were supported as part of the Nanoporous Materials Genome Center by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-FY12-SC0008688.

T.M.M., R.P., L-C.L., J.N., and B.S. were supported as part of the Center for Gas Separations Relevant to Clean Energy Technologies, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE- SC0001015.

A.L.D. thanks the Louise T. Dosdall Fellowship support.
L.-C.L. was supported by the Deutsche Forschungsgemeinschaft (DFG, priority program SPP 1570).

Work at the Molecular Foundry was supported by the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

This research used resources of the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

2. Interpretation of the adsorption experiments

In the main article we compare our mechanism with the adsorption experiments of McDonald *et al.* [1] We argue that the experimental adsorption isotherms are consistent with a chemistry in which 1 CO_2 interacts with 1 amine. As this assumption is different from the conclusions of McDonald *et al.*, [1] it is important to outline our analysis of these experimental adsorption data.

In our analysis we find it useful to replace the unit of loading, which is normally mmol/g, to a unit that is directly related to the chemical structure, i.e., CO_2 molecules/Mg site or CO_2 molecules/amine. To make this conversion we assume that the MOF is a perfect

crystal and that 80% of the Mg sites are covered with an amine and 20% of the sites with water. This gives a conversion factor of 4.25 mmol Mg sites per g material or 3.4 mmol amines per g material. Converted to these units the experimental heats of adsorption are shown in Figures S1 and S2.

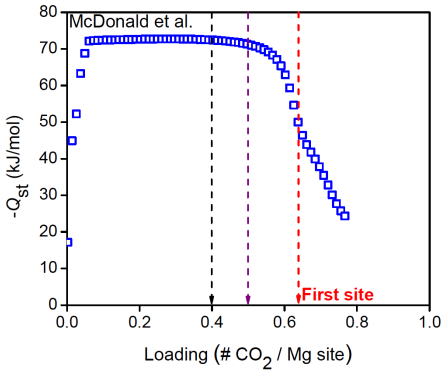

Figure S1: Experimental heat of adsorption as a function of number of adsorbed CO_2 molecules per metal site.

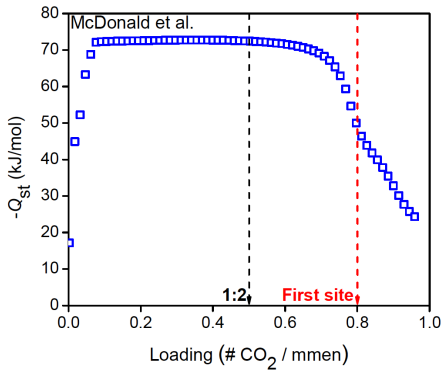

Figure S2: Experimental heat of adsorption as a function of the number of adsorbed CO_2 molecules per mmen.

Two additional assumptions need to be made. The first assumption is related to low heat of adsorption at low loadings. From a thermodynamic point of view this is surprising as in a normal material CO_2 would first adsorb at the sites with the highest binding energy. The fact that CO_2 first adsorbs at sites with relatively low binding energies suggest that at low loading a phase transition occurs. As the crystal structure does not change upon loading of CO_2 such a transition is most likely an ordering of the amines induced by the CO_2. Hence, we need to interpret the data as being two separate isotherms, were the second isotherm has a heat of adsorption of -70 kJ/mol starting from zero loading.

The second assumption is that we have two adsorption sites; the first has a heat of adsorption of -70kJ/mol and the second a heat of adsorption below -25kJ/mol. One would need experimental data at higher loading to determine the heat of adsorption at high loading. The first adsorption site is saturated at the inflection point (see red arrows in Figures S1 and S2).

The conventional chemistry would give a 1:2 stoichiometry, where the adsorption of 1 CO_2 molecule requires two amines. If the stoichiometry would be 1:2 the inflection

would occur at the black arrows in Figures S1 and S2. In the most optimistic scenario that we have a perfect crystal and, not 80%, but all the metals have an amine and all amines would participate in the CO_2 adsorption we would have the purple arrow in Figure S1. Hence, even in a perfect material the coverage of amine should be more than 100% of the metal sites to be consistent with a 1:2 stoichiometry. We feel that this is not a realistic assumption.

If we assume that the stoichiometry is 1:1, we see from figures S1 and S2 that 80% of the amines adsorb CO_2. The fact that not all metal sites carry an amine and that not all amines are accessible for adsorption CO_2 appear to us reasonable assumptions.

The reason that our numbers for the number of CO_2 per amine are different from the interpretation of McDonald *et al.* [1] is that McDonald *et al.* [1] calculated the number of adsorption sites by taking the difference of the lowest and highest loading for which the adsorption enthalpy is -70kJ/mol, which gives a significantly lower loading per amines (65% versus 80%), which would be consistent with a 1:2 stoichiometry in a perfect material.

3. Summary of previously reported mechanisms

The zwitterion mechanism (shown in Figure S3 Eqs. 1-3) is extensively used to describe chemical kinetics observed for the CO_2 capture process in aqueous solutions of primary and secondary alkanolamines, [2-4] This two-step mechanism suggests that the reaction between CO_2 and an amine (denoted here as AmH) proceeds through the formation of a zwitterion as an intermediate which is consecutively deprotonated by a base (B) present in the reaction media. More recently, the so-called termolecular mechanism has been proposed as an alternative mechanism that can also explain the kinetics observed for such systems (Figure S3 Eq. 4). [5-7] In this mechanism the amine bonding to CO_2 and proton transfer to the base (B) take place simultaneously, and the carbamate formation occurs in a single-step reaction. Several researchers claim that the latter mechanism was best-suited

to describe the nature of reactions occurring in these aqueous systems. [5,6,8-10] Nevertheless in both mechanisms, when the role of a base is played by a second amine the overall reaction, which accounts for carbamate/protonated-amine formation in solution, corresponds to an overall 1:2 (CO_2:amine) reaction stoichiometry (Figure S3 Eq. 5). Some recent studies have shown that the main product for the reaction of CO_2 with amines in aprotic polar solvents is free carbamic acid (Figure S3 Eq. 6), whereas in aprotic apolar solvents the same reactants yield the precipitation of the corresponding [carbamate][ammonium] salt (Figure S3 Eq. 7). [11,12]

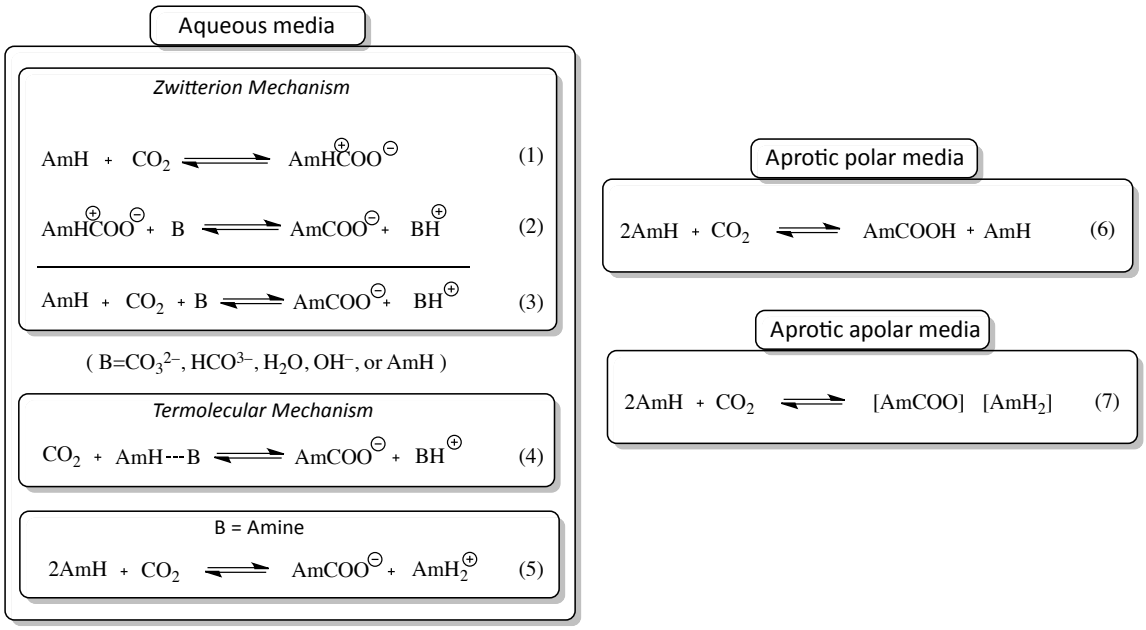

Figure S3: Different reactivity currently proposed for amine CO_2 reaction in solution. In the zwitterion mechanism, the Am-C bond formation occurs followed by deprotonation by a base, while in the termolecular mechanism the base abstracts the proton during formation of the Am-C bond. Both aqueous media proposed mechanisms result in the carbamate + protonated base products. In aprotic polar media, the products are predicted to be neutral acid + amine species, while in aprotic apolar media, the product is predicted as a [carbamate][ammonium] salt.

4. Computational details

Periodic System Calculations. The initial periodic structures for Mg_2(dobpdc) and the amine-loaded (1amine:1metal) mmen-Mg_2(dobpdc) were optimized using the SIESTA package[13,14] and the PBE functional[15-17] with the Grimme correction[18,19] which was employed to account for long-ranged dispersion forces. Recent work[20,21] shows that this method correctly predicts the experimental heat of adsorption of CO_2 in MOFs. Norm-conserving Trouiller-Martin pseudopotentials[22] are used in calculations. 2s and 2p electrons of C, N, and O atoms are explicitely included in the valence; for Mg, semicore electrons are considered (2s, 2p, and 3s). We use a variationally optimized[23] double-ζ polarized basis set including d-orbitals for all atoms. The integration over the Brillouin zone is carried over 64 grid points.[24] Real space integrals are performed on a mesh with a 280 Ry cutoff. For each calculation, atomic positions of all atoms are optimized until forces are smaller than 40 meV/Ang. Vibrational frequencies are computed at the Gamma point on optimized structure (forces < 10 meV/Å) from a dynamical matrix obtained through a finite difference approach.

Fragment System Calculations. From the initial Mg_2(dobpdc) periodic structure, two small MOF model fragments were chosen for the mechanistic study. The AB-fragment was designed to study amine interactions across the organic linker, while the C-fragment was designed to study interactions along the axis containing a row of open-metal sites. Protons were used to cap the fragments and maintain neutral charge, see Figure 1. The **C-axis-fragment**; contains 106 atoms consisting of 6 Mg atoms, 7 truncated linkers and 2 additional protons (to maintain a neutral total charge). The **AB-plane-fragment** contains 206 atoms total consisting of 12 metal sites, three full linkers, and 8 truncated linkers and 2 additional protons (to maintain a neutral total charge).

For the mechanistic study, constrained optimizations were performed where the geometry of the MOF fragment was kept rigid, while the mmen, CO_2, and derived species were fully relaxed. Geometry optimizations were performed using PBE[15-17] + D[18,19] with the Ahlrich's basis sets.[25,26] The effect due to relaxation of the Mg and neighbor O atoms of the framework was investigated. For all mmen and CO_2, def-TZVP was used, while for the MOF fragment atoms, the following were used: Mg, def-TZVPP; O, def-TZVP; C,

def-SV(P); H, def-SV(P). The effect of counterpoise (CP) basis set superposition error (BSSE) corrections was investigated. Stationary points were verified by numerical frequency calculations. All fragment model calculations used the Turbomole 6.4 software package. [27]

The CP correction for BSSE reported in table S4 (section 7 of this SI) is shown below:

$$\Delta E_{AB}^{CP} = E_{AB}(AB) + \left[E_A(A) - E_A(AB)\right] + \left[E_B(B) - E_B(AB)\right] - E_A^0(A) - E_B^0(B)$$

where $E_{AB}(AB)$ is the dimer energy in the basis of the dimer, $\left[E_A(A) - E_A(AB)\right]$ is the energy difference between monomer A (in the basis of A) and monomer A (in the basis of AB), $\left[E_B(B) - E_B(AB)\right]$ is the energy difference between monomer B (in the basis of B) and monomer B (in the basis of AB), $E_A^0(A)$ is the energy of monomer A in the basis of A in the original geometry of monomer A, and $E_B^0(B)$ is the energy of monomer B in the basis of B in the original geometry of monomer B.

For all species, $E_B^0(B)$ is given by the energy of CO_2 in the geometry of isolated (gas phase) CO_2. For species A_{II}-B_{II}, $E_A^0(A)$ is given by the energy of species A_I in the A_I geometry. For species B_{III}-C_{II}, $E_A^0(A)$ is given by the energy of species B_{II} in the B_{II} geometry.

5. Functional Survey

To discard a computational artifact yielding the neutral carbamic acid species instead of carbamate:amoinum salt due to functional dependence on the description of H-bond interactions, as had been previously reported for similar systems[11] , a brief study of the carbamate:protonated amine (or carbamic acid :amine) analogous to B_{II} without the fragment (Figure S4) was performed.

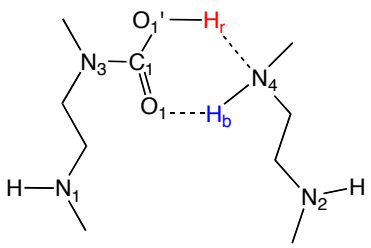

Figure S4. Atom labeling scheme of the studied species.

We performed this study using the following functionals: The 1996 functional of Perdew, Burke and Ernzerhof (PBE) [16,17,28], its 1998 revision (PBEh) [29], and its hybrid version (25% exchange and 75% correlation) by Adamo[30]. For the M06-class functionals, the pure functional of Truhlar and Zhao (M06L) [31]and the hybrid (M062X) [32]. Of a third family, the correlation functionals of Lee, Yang, and Parr BLYP[33,34]and B3LYP[33,35-37]. Finally, the long range corrected functionals LC-wPBE by Scuseria[38-40]and CAM-B3LYP[41] Handy and coworkers' long range corrected version of B3LYP using the Coulomb-attenuating method. As can be seen in Table S1, all functionals tested yielded the same product in the gas phase; carbamic acid H-bound to an amine.

Table S1. Summary of most relevant distances and angles of the optimized species using different functionals.

Distance or angle/ Functional	PBE	PBE0	PBEh	LC-wPBE	BLYP	B3LYP	CAM-B3LYP	M06L	M06-2X
N_3-C_1	1.38	1.37	1.38	1.36	1.38	1.37	1.36	1.37	1.36
C_1-O_1	1.25	1.23	1.25	1.23	1.25	1.23	1.23	1.23	1.23
C_1-$O_{1'}$	1.35	1.33	1.35	1.33	1.36	1.34	1.34	1.34	1.34
$O_{1'}$-H_r	1.05	1.02	1.05	1.02	1.04	1.02	1.02	1.01	1.02
O_1-H_b	2.06	2.11	2.04	2.14	2.14	2.16	2.11	2.29	2.21
N_4-H_r	1.63	1.66	1.64	1.68	1.70	1.71	1.69	1.74	1.68
H_4-H_b	1.04	1.02	1.04	1.02	1.03	1.02	1.02	1.02	1.02
O_1-C_1-$O_{1'}$	124.2	123.8	124.2	123.6	123.9	123.6	123.5	124.0	123.7
H_b-N_4-H_r	86.1	86.5	85.7	85.8	85.63	85.8	85.7	90.6	89.7

6. Detailed structural parameters

6.1. Selected distances and angles for the different species in the mechanism

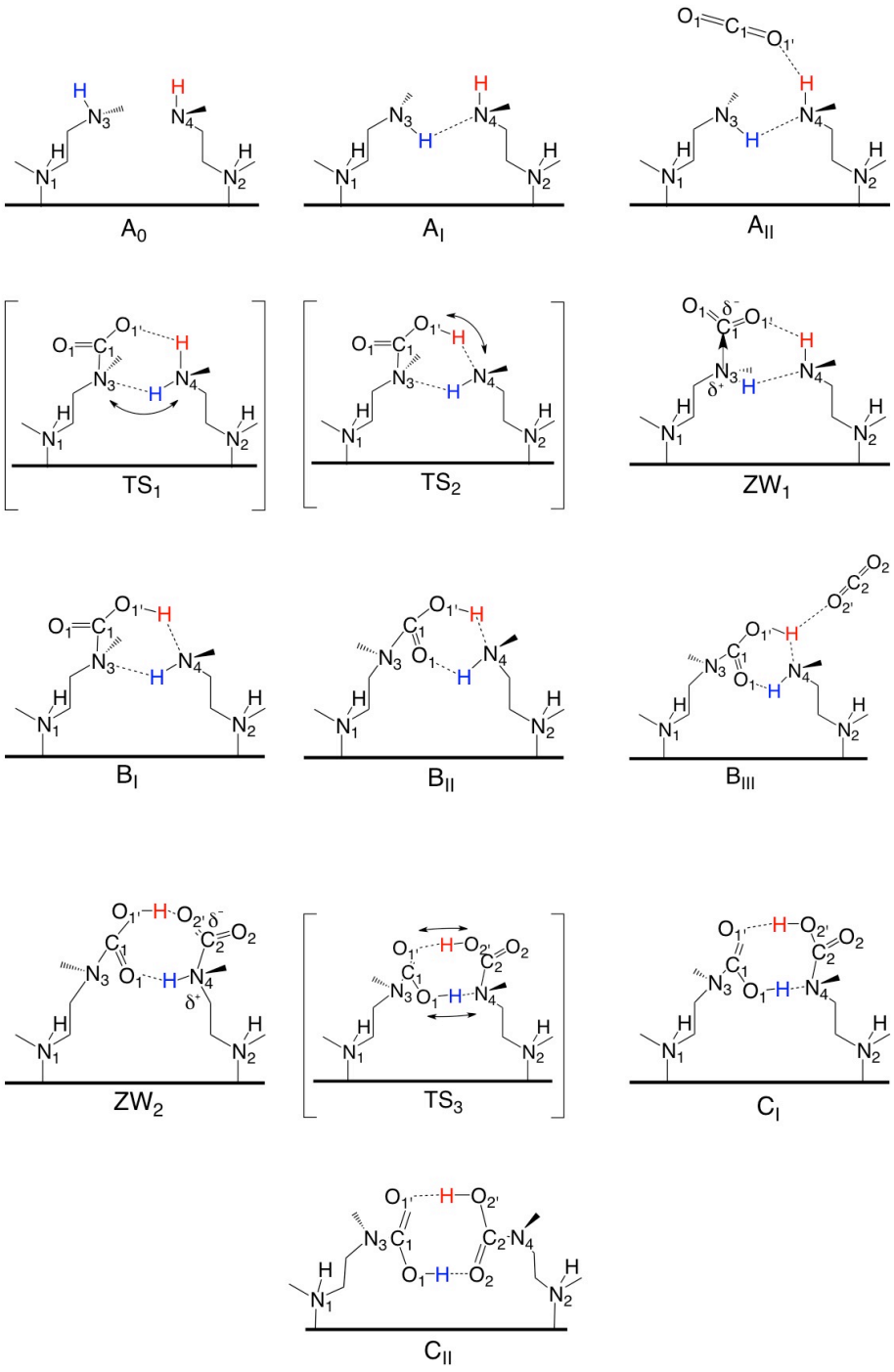

Figure S5. Atom labeling scheme for the different species.

Table S2. Relevant structural parameters for Fragment-C Species. Labels adopted from Figure S5, where Hb and Hr are the blue and red H atoms, respectively.

Species / Dist/Angle	A_0	A_I	A_{II}	ZW_I	B_I	B_{II}	B_{III}	ZW_{II}	C_I	C_{II}

Mg N_1	2.26	2.27	2.26	2.3	2.3	2.37	2.31	2.25	2.25	2.25
Mg N_2	2.27	2.29	2.29	2.28	2.28	2.28	2.29	2.31	2.32	2.32
N_3 Hb	1.02	1.03	1.03	1.04	2.47	3.76	3.83	3.71	3.1	3.07
N_3 Hr	5.18	3.51	3.18	2.91	2.44	3.1	3.1	3.11	3.72	3.25
N_4 Hb	4.28	2.2	2.23	2.03	1.03	1.03	1.03	1.05	1.53	3.43
N_4 Hr	1.02	1.02	1.02	1.02	1.67	1.71	1.66	3.15	2.45	3.09
N_3 C_1			5.93	2.17	1.4	1.37	1.37	1.36	1.36	1.36
Hr $O_{1'}$			2.37	2.29	1.03	1.03	1.04	1.01	1.58	1.93
Hb O_1			6.8	3.2	3.68	2.14	2.16	1.66	1.06	0.99
$O_{1'}$-C_1			1.17	1.2	1.35	1.35	1.35	1.34	1.25	1.24
C_1-O_1			1.17	1.19	1.22	1.24	1.24	1.25	1.34	1.36
O_1-C_1-$O_{1'}$			179.9	155.5	122.4	123.7	123.3	123.9	123.4	123.2
Hr $O_{2'}$							3.05	1.7	1.03	0.99
Hb O_2							6.53	3.17	3.59	1.91
N_4 C_2							4.39	1.74	1.47	1.36
C_2 $O_{2'}$							1.17	1.23	1.33	1.36
C_2 O_2							1.17	1.21	1.21	1.24
O_2-C_2-$O_{2'}$							179.7	141	124.7	122.8

6.2. Discussion of key structural parameters of ZW_1, ZW_2 and C_{II} .

As illustrated in Figure S6-A and S6-B, in ZW_1 not only the N-CO_2 bond length is substantially longer than in ZW_2 (2.19 and 1.74 A respectively) but the two H-bond distances are very different (2.30 and 2.03 Å, respectively), whereas in ZW_2 the fact that both H-bonds are approximately 1.70 Å promotes the concerted transition (TS3).

As reported in Figure 2 of the main text, the formation of B_{II} from A_I is -29.76 kJ/CO_2 mol and the energy of formation of C_{II} in the C-fragment is -35 kJ/ CO_2 mol (-70 kJ/mol in Figure 2 when two CO_2 are adsorbed). Most importantly, the isomerization from C_I in the C-fragment to C_{II} in the AB-fragment occurs due to the optimum spatial arrangement for a double H bond across the linker (Figure S6-C). The distance between the two Mg which coordinate N1 and N3 (labeling scheme in Figure S5) place the two carbamic acid functionalities (O=C_1-OH and O=C_2-OH) in the arrangement for a "head to tail" interaction. This critical isomerization step contributes to half of the total energy of

formation from A_I to C_{II}, which is -69.13 kJ/ CO_2 mol (-138.25 kJ/mol in Figure 2 where two CO_2 are adsorbed).

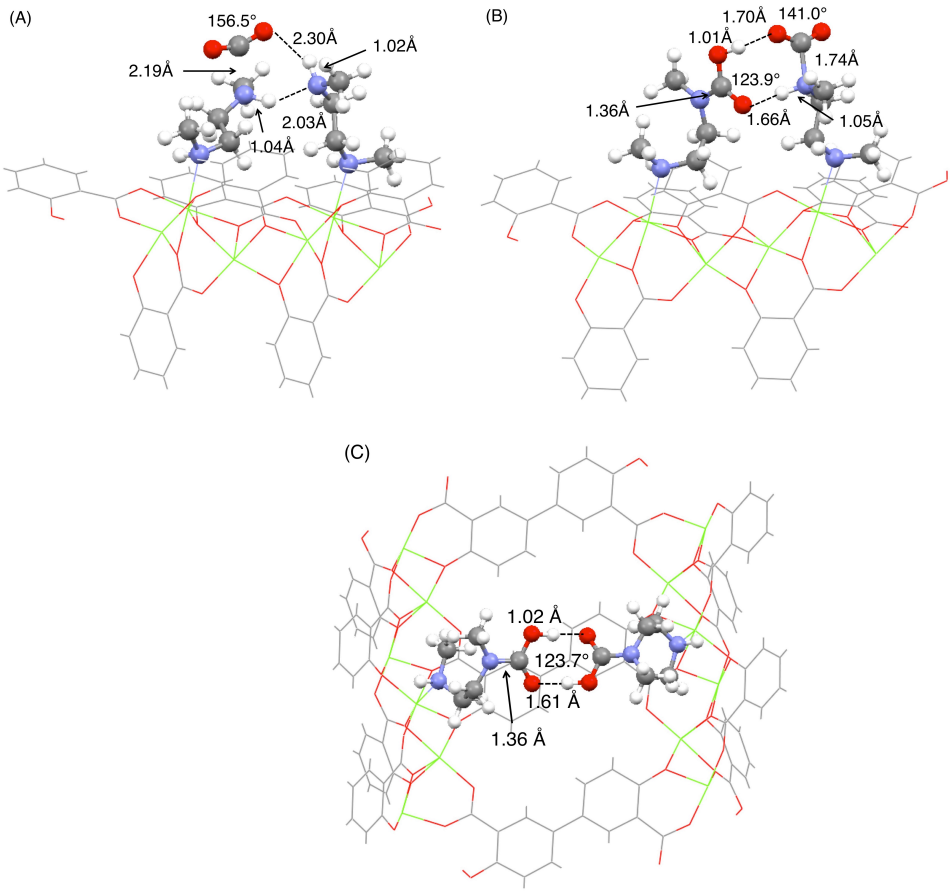

Figure S6. View of key fragment species with highlighted critical structural parameters. A) ZW_1, B) ZW_2 and C) C_{II} (in the AB-fragment). Framework atoms are shown as wireframe and the amine:CO_2-derived species with ball and stick. Color code: Mg, green; C, grey; H, white; N, blue; O, red.

6.2. Mg-N distances upon relaxation of Mg and O atoms of the framework.

For all of the minimum energy species shown in Figure S5, optimizations were performed where the Mg and 5 nearest neighbor O atoms of the framework were allowed to relax, in addition to the mmen and CO_2 species. In all cases, this relaxation resulted in a shortening of the Mg-N bond accompanied by a lowering of the absolute energy by ca. 0.2 a.u. The energetics of the framework atom relaxation are discussed in Section S7.

Table S3. Comparison of the Mg-N distances for selected Fragment-C Species upon keeping the coordinates of all the framework atoms fixed (standard) vs allowing the Mg and O of the framework to relax (relaxed). Labels adopted from Figure S5, where Hb and Hr are the blue and red H atoms, respectively.

Species \ Distance	standard		relaxed	
	Mg-N_1	**Mg-N_2**	**Mg-N_1**	**Mg-N_2**
A_0	2.27	2.27	2.21	2.20
A_I	2.27	2.29	2.22	2.21
A_{II}	2.26	2.29	2.20	2.22
ZW_I	2.30	2.28	2.23	2.21
B_I	2.30	2.28	2.23	2.22
B_{II}	2.37	2.28	2.23	2.21
B_{III}	2.31	2.29	2.24	2.24
ZW_{II}	2.25	2.31	2.21	2.24
C_I	2.25	2.32	2.21	2.24
C_{II}	2.25	2.33	2.20	2.25

7. Energies of optimized species

Below we report the energies of the different species involved in the mechanistic study shown in the main text, where the positions of the atoms of the MOF-framework were kept fixed (column A, table S4). To investigate the effects of the frozen atom approach for the MOF fragment, the energy profile upon relaxation of the metal centers and their first coordination sphere O atoms are reported (column B, table S4). The effects on the energy profile of the inclusion of BSSE by CP correction was also considered (column C, table S4).

Table S4. Energy of the different species from the different cluster models (A), upon relaxation of the Mg and O atoms of the framework (B) and upon BSSE correction (C).

Fragment	Species	A	B	C
		dE (kJ/mol)[a]	dE relax Mg,O (kJ/mol)[b]	dE CP (kJ/mol)[c]
C-axis	A_0	+15.40	+15.20	---
	A_I	0.00	0.00	0.00
	A_{II}	+4.73	-2.76	+5.88
	ZW_I	-19.58	-18.75	-14.81
	TS_1	+18.01	---	+27.46
	TS_2	-15.32	---	-6.01
	B_I	-15.76	-14.10	-6.09
	B_{II}	-29.76	-30.93	-19.50
	B_{III}	-33.83	-44.28	-22.27
	ZW_2	-68.63	-65.60	-49.70
	TS_3	-28.25	---	-9.26
	C_I	-41.99	-40.72	-23.36
	C_{II}	-70.05	-68.09	-49.61
AB-plane	A_0	+15.40	---	---
	$A_{I'}$	+59.59	---	---
	C_{II}	-138.25	---	---

[a] All the positions of the atoms of the MOF-framework were kept frozen for the optimization. [b] The Mg and O atoms of the framework were allowed to relax together with the amines and CO_2 molecules or derived species. [c] Energies corresponding to the optimized species maintaining the whole MOF-framework frozen but corrected for BSSE by CP inclusion.

In column A of Table S4, for consistency of the energies of the species obtained with the

two fragment models, A_0(AB-plane) was set as energy +15.40 kJ/mol as is the energy of the analogous A_0(C-axis) with respect to A_I(C-axis) since the latter is the global lowest energy conformation for the amines. The corresponding A_I(AB-plane) cannot be computed due to limitations of the fragment that does not allow the presence of two neighboring amines along the C-axis. Further, as discussed in the main text, the $A_{I'}$(AB-plane) structure where the two amines are H-bound across the linker are higher in energy than the non interacting amines in A_0(AB-plane) structure.

As can be seen in column B of Table S4, when the framework Mg and 5 nearest neighbor O atoms were allowed to relax, the overall picture of the mechanism did not change significantly. The major notable difference is that the initial H-bonded CO_2 species (A_{II} and B_{III}) were stabilized significantly more by this geometric flexibility than were the other species.

Introducing basis set superposition error in a study like the one reported herein involving reactive species and transition structures can lead to unphysical data.[42] However, the effect of BSSE, column C of Table S4, was investigated for some selected species. The magnitude of the correction is shown in table S4 for a given fragment choice, and is noted that while all species are destabilized by the CP correction, the overall mechanistic picture does not change.

7. Computed IR frequencies

In Figure S7 we report the IR stretches calculated for the products B_{II} and C_{II}. Our computed stretches for B_{II} and C_{II} could both match the experimental spectra. Thus, IR spectroscopy has proven to not be a definitive tool to prove/deny the proposed mechanism. Current efforts are devoted in finding a suitable spectroscopy to verify the proposed mechanism.

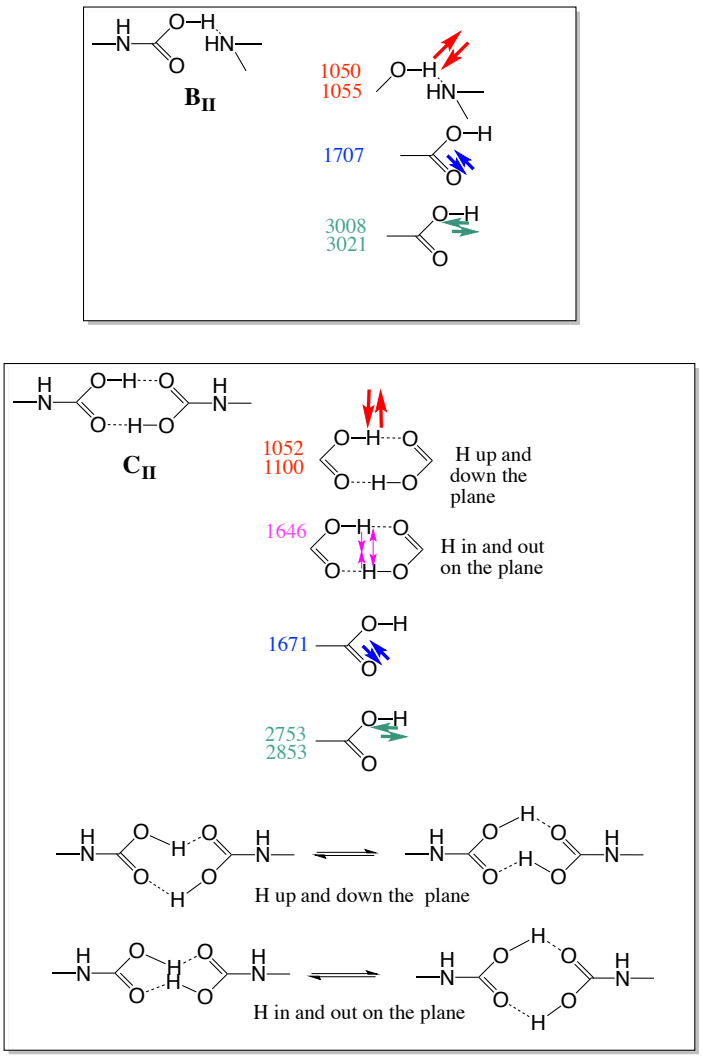

Figure S7. Computed IR stretches involving the H-bound moieties in B_{II} and C_{II}.

8. Coordinates of optimized species

==========

A_0(C-axis)

==========

142

ENERGY = -5199.148863861

N	30.816370	4.242608	7.459783
C	29.728453	4.161815	8.461463
H	30.181194	4.224703	9.459906
C	28.889461	2.889653	8.423300
H	28.209386	2.906971	9.309437
H	29.556262	2.022308	8.573715
N	28.155448	2.689354	7.177728
H	27.621779	3.535535	6.963845
C	27.256836	1.543306	7.253127
H	26.555989	1.580543	8.117808
H	26.667949	1.465372	6.327520
H	27.852895	0.621218	7.352656
H	29.096156	5.054077	8.327507
H	31.270154	3.322264	7.435768
C	30.331375	4.561235	6.097519
H	31.168983	4.914585	5.488959
H	29.818313	3.708950	5.627584
H	29.626286	5.400768	6.173328

N	30.840662	4.147374	14.611615
C	29.700252	4.187473	15.548154
H	30.090311	4.224107	16.572581
H	29.116168	5.098756	15.363028
H	29.037184	3.309863	15.439044
C	30.405546	3.979217	13.207919
H	31.149100	4.431942	12.541452
C	30.226270	2.498468	12.878093
H	29.568526	2.033390	13.650040
H	31.211894	2.008650	12.963023
N	29.741453	2.273463	11.524307
H	28.832984	2.729980	11.408242
C	29.609921	0.846884	11.239926
H	28.995761	0.297941	11.987656
H	29.158872	0.703343	10.247806
H	30.613938	0.392793	11.235293
H	31.393064	3.316626	14.859548
H	29.463916	4.535478	13.069152
Mg	34.197003	6.437400	5.842800
O	31.310702	8.053301	4.968900
O	33.750003	4.620000	6.770501
O	32.357202	6.930901	6.633101
O	32.580103	4.066100	2.644600
O	33.076103	5.541300	4.284200
H	29.072902	8.746601	5.503900
H	34.237903	0.099700	7.002901
H	33.102303	1.789000	3.173900
C	33.682703	3.392000	6.164300
C	29.028302	8.466801	6.557501
C	33.972003	0.951900	6.370000
C	33.962203	2.229200	6.938301
C	31.331202	7.604501	6.177200
C	33.360003	3.196800	4.768300
C	33.370103	1.884600	4.227500
C	32.980703	4.311100	3.845000
Mg	32.561103	5.495400	8.196001
Mg	34.197603	6.437100	12.862301
Mg	32.569403	7.387801	10.519601
O	31.217502	6.788601	9.097901
O	33.912903	6.852001	8.987001
O	31.311302	8.053001	11.988401
O	33.750503	4.619700	13.790001
O	32.357802	6.930501	13.652601
O	32.580603	4.065800	9.664101
O	34.358003	7.918101	11.447401
O	33.076603	5.541000	11.303701
O	35.399503	7.199101	7.316701
H	29.073402	8.746301	12.523401
H	34.181503	2.365100	8.001001
H	34.238403	0.099400	14.022401
H	33.102903	1.788600	10.193401
H	38.031803	10.595001	11.686301
H	36.093003	9.414401	12.680101
H	37.131403	8.785501	7.849201
H	27.059102	8.618701	9.342801
H	29.057302	7.535301	10.336901
C	33.683303	3.391600	13.183801
C	30.174402	7.829701	7.097601
C	29.028802	8.466401	13.577001
C	33.972603	0.951600	13.389501
C	33.962803	2.228800	13.957801
C	31.331802	7.604201	13.196701
C	35.453503	8.475701	10.840901
C	33.360603	3.196500	11.787801
C	33.370603	1.884300	11.247001
C	37.422803	9.944701	11.050701
C	36.321503	9.296401	11.617201
C	32.981303	4.310800	10.864501
C	30.185302	7.456801	8.494201
C	35.781803	8.299301	9.443201
C	36.912403	8.967301	8.902701
C	37.746503	9.802701	9.667901
C	27.927802	8.417201	8.708501
C	29.042102	7.792401	9.274201
C	35.005503	7.408101	8.525501
Mg	32.570003	7.387501	17.539101
O	31.218102	6.788201	16.117401
O	33.862403	6.902701	16.002901
O	33.751103	4.619300	20.809502
O	32.581203	4.065400	16.683601
O	34.358603	7.917801	18.466901
O	33.077203	5.540600	18.323201

O	35.400003	7.198801	14.336201
H	34.182003	2.364800	15.020401
H	34.239003	0.099100	21.041902
H	33.103403	1.788300	17.212901
H	38.032403	10.594701	18.705701
H	36.093503	9.414101	19.699602
H	37.132003	8.785201	14.868701
H	27.059702	8.618401	16.362301
H	29.057902	7.535001	17.356401
C	33.683803	3.391300	20.203302
C	30.175002	7.829401	14.117101
C	33.973103	0.951300	20.409002
C	33.963303	2.228500	20.977302
C	35.454103	8.475401	17.860401
C	33.361103	3.196200	18.807301
C	33.371203	1.884000	18.266501
C	37.423303	9.944401	18.070201
C	36.322103	9.296101	18.636701
C	32.981903	4.310500	17.884001
C	30.185802	7.456401	15.513701
C	35.782403	8.299001	16.462701
C	36.913003	8.967001	15.922201
C	37.747003	9.802401	16.687301
C	27.928402	8.416801	15.728001
C	29.042602	7.792001	16.293701
C	35.006103	7.407801	15.545001
H	38.612603	10.315201	16.242001
H	38.612003	10.314701	9.222401
H	33.601403	5.288800	20.060302
H	32.413202	3.096700	2.517700
H	34.215303	2.370900	22.039902
Mg	32.561703	5.495100	15.215501
C	33.679003	0.743400	4.989000
H	33.690503	-0.229000	4.542700
C	33.679603	0.743100	12.008501
H	33.691103	-0.229300	11.562201
C	33.680103	0.742800	19.028001
H	33.691603	-0.229600	18.581701
C	27.890302	8.765101	14.345401
H	27.037702	9.234001	13.900301
C	27.889702	8.765401	7.325901
H	27.037002	9.234101	6.880801

==========

A_I(C-axis)

==========

142

ENERGY = -5199.154729390

N	30.800527	4.221175	7.478618
C	29.748762	4.186459	8.516437
H	30.230393	3.959725	9.476392
C	28.625077	3.174737	8.279663
H	29.054816	2.159689	8.233987
H	28.124666	3.375403	7.307070
N	27.669465	3.215852	9.397255
H	27.064918	2.394813	9.338743
C	26.831004	4.420246	9.384330
H	26.338425	4.598281	8.404333
H	26.055215	4.329094	10.158292
H	27.437505	5.308005	9.614504
H	29.324383	5.196324	8.571305
H	31.248992	3.298643	7.454488
C	30.275636	4.541954	6.135975
H	31.096593	4.864893	5.486907
H	29.733286	3.701393	5.669187
H	29.586980	5.393135	6.228986
N	30.830331	4.163238	14.587094
C	29.686689	4.184856	15.520407
H	30.073536	4.199591	16.547010
H	29.105255	5.101329	15.352815
H	29.021726	3.312100	15.390213
C	30.406809	4.043465	13.173499
H	31.171817	4.497109	12.533022
C	30.204182	2.579460	12.779997
H	29.420189	2.125268	13.432323
H	31.147303	2.046031	13.001989
N	29.935663	2.409934	11.363494
H	29.061512	2.867281	11.069957
C	29.877003	1.004577	10.989748
H	29.132132	0.411905	11.568637
H	29.627920	0.916571	9.921203
H	30.865875	0.543669	11.151295
H	31.375050	3.320857	14.811000

H	29.482722	4.628021	13.037726
Mg	34.197003	6.437400	5.842800
O	31.310702	8.053301	4.968900
O	33.750003	4.620000	6.770501
O	32.357202	6.930901	6.633101
O	32.580103	4.066100	2.644600
O	33.076103	5.541300	4.284200
H	29.072902	8.746601	5.503900
H	34.237903	0.099700	7.002901
H	33.102303	1.789000	3.173900
C	33.682703	3.392000	6.164300
C	29.028302	8.466801	6.557501
C	33.972003	0.951900	6.370000
C	33.962203	2.229200	6.938301
C	31.331202	7.604501	6.177200
C	33.360003	3.196800	4.768300
C	33.370103	1.884600	4.227500
C	32.980703	4.311100	3.845000
Mg	32.561103	5.495400	8.196001
Mg	34.197603	6.437100	12.862301
Mg	32.569403	7.387801	10.519601
O	31.217502	6.788601	9.097901
O	33.912903	6.852001	8.987001
O	31.311302	8.053001	11.988401
O	33.750503	4.619700	13.790001
O	32.357802	6.930501	13.652601
O	32.580603	4.065800	9.664101
O	34.358003	7.918101	11.447401
O	33.076603	5.541000	11.303701
O	35.399503	7.199101	7.316701
H	29.073402	8.746301	12.523401
H	34.181503	2.365100	8.001001
H	34.238403	0.099400	14.022401
H	33.102903	1.788600	10.193401
H	38.031803	10.595001	11.686301
H	36.093003	9.414401	12.680101
H	37.131403	8.785501	7.849201
H	27.059102	8.618701	9.342801
H	29.057302	7.535301	10.336901
C	33.683303	3.391600	13.183801
C	30.174402	7.829701	7.097601
C	29.028802	8.466401	13.577001
C	33.972603	0.951600	13.389501
C	33.962803	2.228800	13.957801
C	31.331802	7.604201	13.196701
C	35.453503	8.475701	10.840901
C	33.360603	3.196500	11.787801
C	33.370603	1.884300	11.247001
C	37.422803	9.944701	11.050701
C	36.321503	9.296401	11.617201
C	32.981303	4.310800	10.864501
C	30.185302	7.456801	8.494201
C	35.781803	8.299301	9.443201
C	36.912403	8.967301	8.902701
C	37.746503	9.802701	9.667901
C	27.927802	8.417201	8.708501
C	29.042102	7.792401	9.274201
C	35.005503	7.408101	8.525501
Mg	32.570003	7.387501	17.539101
O	31.218102	6.788201	16.117401
O	33.862403	6.902701	16.002901
O	33.751103	4.619300	20.809502
O	32.581203	4.065400	16.683601
O	34.358603	7.917801	18.466901
O	33.077203	5.540600	18.323201
O	35.400003	7.198801	14.336201
H	34.182003	2.364800	15.020401
H	34.239003	0.099100	21.041902
H	33.103403	1.788300	17.212901
H	38.032403	10.594701	18.705701
H	36.093503	9.414101	19.699602
H	37.132003	8.785201	14.868701
H	27.059702	8.618401	16.362301
H	29.057902	7.535001	17.356401
C	33.683803	3.391300	20.203302
C	30.175002	7.829401	14.117101
C	33.973103	0.951300	20.409002
C	33.963303	2.228500	20.977302
C	35.454103	8.475401	17.860401
C	33.361103	3.196200	18.807301
C	33.371203	1.884000	18.266501
C	37.423303	9.944401	18.070201
C	36.322103	9.296101	18.636701
C	32.981903	4.310500	17.884001

C	30.185802	7.456401	15.513701
C	35.782403	8.299001	16.462701
C	36.913003	8.967001	15.922201
C	37.747003	9.802401	16.687301
C	27.928402	8.416801	15.728001
C	29.042602	7.792001	16.293701
C	35.006103	7.407801	15.545001
H	38.612603	10.315201	16.242001
H	38.612003	10.314701	9.222401
H	33.601403	5.288800	20.060302
H	32.413202	3.096700	2.517700
H	34.215303	2.370900	22.039902
Mg	32.561703	5.495100	15.215501
C	33.679003	0.743400	4.989000
H	33.690503	-0.229000	4.542700
C	33.679603	0.743100	12.008501
H	33.691103	-0.229300	11.562201
C	33.680103	0.742800	19.028001
H	33.691603	-0.229600	18.581701
C	27.890302	8.765101	14.345401
H	27.037702	9.234001	13.900301
C	27.889702	8.765401	7.325901
H	27.037002	9.234101	6.880801

==========

A_{II}(C-axis)

==========

145

ENERGY = -5387.622194963

C	25.494518	0.021649	7.836419
O	26.040686	0.580128	8.711684
O	24.951736	-0.536549	6.962741
N	30.801077	4.213133	7.494660
C	29.734613	4.210950	8.518074
H	30.203590	4.036312	9.495015
C	28.594847	3.209865	8.311608
H	28.952907	2.185275	8.509073
H	28.240042	3.247215	7.257871
N	27.516019	3.509776	9.256542
H	26.931420	2.681483	9.364256
C	26.681978	4.642134	8.846545
H	26.274655	4.534125	7.817255
H	25.842672	4.743166	9.549481
H	27.258817	5.578567	8.879956
H	29.316085	5.224118	8.536611
H	31.240232	3.286250	7.481893
C	30.294845	4.532567	6.143877
H	31.125033	4.859373	5.509018
H	29.763264	3.691057	5.667447
H	29.602502	5.381755	6.226065
N	30.852540	4.187765	14.513927
C	29.753771	4.058319	15.493730
H	30.185265	3.912559	16.491195
H	29.169003	4.988364	15.488304
H	29.078498	3.218359	15.250092
C	30.318353	4.230079	13.130269
H	31.087835	4.672386	12.486128
C	29.880796	2.843030	12.616576
H	29.935391	2.131687	13.462228
H	30.617552	2.473987	11.867157
N	28.506826	2.805845	12.123509
H	28.389519	3.417827	11.304129
C	28.142462	1.456842	11.710866
H	28.135530	0.789229	12.589033
H	27.130453	1.457102	11.281107
H	28.839207	1.010876	10.961824
H	31.417465	3.331704	14.591073
H	29.453996	4.911988	13.130789
Mg	34.197003	6.437400	5.842800
O	31.310702	8.053301	4.968900
O	33.750003	4.620000	6.770501
O	32.357202	6.930901	6.633101
O	32.580103	4.066100	2.644600
O	33.076103	5.541300	4.284200
H	29.072902	8.746601	5.503900
H	34.237903	0.099700	7.002901
H	33.102303	1.789000	3.173900
C	33.682703	3.392000	6.164300
C	29.028302	8.466801	6.557501
C	33.972003	0.951900	6.370000
C	33.962203	2.229200	6.938301
C	31.331202	7.604501	6.177200
C	33.360003	3.196800	4.768300
C	33.370103	1.884600	4.227500

C	32.980703	4.311100	3.845000
Mg	32.561103	5.495400	8.196001
Mg	34.197603	6.437100	12.862301
Mg	32.569403	7.387801	10.519601
O	31.217502	6.788601	9.097901
O	33.912903	6.852001	8.987001
O	31.311302	8.053001	11.988401
O	33.750503	4.619700	13.790001
O	32.357802	6.930501	13.652601
O	32.580603	4.065800	9.664101
O	34.358003	7.918101	11.447401
O	33.076603	5.541000	11.303701
O	35.399503	7.199101	7.316701
H	29.073402	8.746301	12.523401
H	34.181503	2.365100	8.001001
H	34.238403	0.099400	14.022401
H	33.102903	1.788600	10.193401
H	38.031803	10.595001	11.686301
H	36.093003	9.414401	12.680101
H	37.131403	8.785501	7.849201
H	27.059102	8.618701	9.342801
H	29.057302	7.535301	10.336901
C	33.683303	3.391600	13.183801
C	30.174402	7.829701	7.097601
C	29.028802	8.466401	13.577001
C	33.972603	0.951600	13.389501
C	33.962803	2.228800	13.957801
C	31.331802	7.604201	13.196701
C	35.453503	8.475701	10.840901
C	33.360603	3.196500	11.787801
C	33.370603	1.884300	11.247001
C	37.422803	9.944701	11.050701
C	36.321503	9.296401	11.617201
C	32.981303	4.310800	10.864501
C	30.185302	7.456801	8.494201
C	35.781803	8.299301	9.443201
C	36.912403	8.967301	8.902701
C	37.746503	9.802701	9.667901
C	27.927802	8.417201	8.708501
C	29.042102	7.792401	9.274201
C	35.005503	7.408101	8.525501
Mg	32.570003	7.387501	17.539101
O	31.218102	6.788201	16.117401
O	33.862403	6.902701	16.002901
O	33.751103	4.619300	20.809502
O	32.581203	4.065400	16.683601
O	34.358603	7.917801	18.466901
O	33.077203	5.540600	18.323201
O	35.400003	7.198801	14.336201
H	34.182003	2.364800	15.020401
H	34.239003	0.099100	21.041902
H	33.103403	1.788300	17.212901
H	38.032403	10.594701	18.705701
H	36.093503	9.414101	19.699602
H	37.132003	8.785201	14.868701
H	27.059702	8.618401	16.362301
H	29.057902	7.535001	17.356401
C	33.683803	3.391300	20.203302
C	30.175002	7.829401	14.117101
C	33.973103	0.951300	20.409002
C	33.963303	2.228500	20.977302
C	35.454103	8.475401	17.860401
C	33.361103	3.196200	18.807301
C	33.371203	1.884000	18.266501
C	37.423303	9.944401	18.070201
C	36.322103	9.296101	18.636701
C	32.981903	4.310500	17.884001
C	30.185802	7.456401	15.513701
C	35.782403	8.299001	16.462701
C	36.913003	8.967001	15.922201
C	37.747003	9.802401	16.687301
C	27.928402	8.416801	15.728001
C	29.042602	7.792001	16.293701
C	35.006103	7.407801	15.545001
H	38.612603	10.315201	16.242001
H	38.612003	10.314701	9.222401
H	33.601403	5.288800	20.060302
H	32.413202	3.096700	2.517700
H	34.215303	2.370900	22.039902
Mg	32.561703	5.495100	15.215501
C	33.679003	0.743400	4.989000
H	33.690503	-0.229000	4.542700
C	33.679603	0.743100	12.008501
H	33.691103	-0.229300	11.562201

C	33.680103	0.742800	19.028001
H	33.691603	-0.229600	18.581701
C	27.890302	8.765101	14.345401
H	27.037702	9.234001	13.900301
C	27.889702	8.765401	7.325901
H	27.037002	9.234101	6.880801

==========

ZW_1(C-axis)

==========

145

ENERGY= -5387.631451817

C	27.298500	1.541600	12.687000
O	26.719500	1.218800	11.692200
O	27.413300	1.760100	13.852300
N	30.797800	4.227500	7.495000
C	29.761700	4.245700	8.544700
H	30.264500	4.198200	9.519400
C	28.714100	3.134700	8.484500
H	29.217900	2.152500	8.494900
H	28.124600	3.206200	7.544700
N	27.869400	3.224300	9.678100
H	27.330800	2.364800	9.803900
C	26.950600	4.366200	9.666200
H	26.352000	4.428300	8.733100
H	26.263800	4.276900	10.519500
H	27.507000	5.309700	9.769700
H	29.265700	5.222000	8.484000
H	31.234500	3.298700	7.491800
C	30.250500	4.509700	6.152900
H	31.067800	4.760400	5.468200
H	29.654900	3.674800	5.744100
H	29.608000	5.398100	6.222600
N	30.820800	4.115900	14.608600
C	29.704000	4.160800	15.581000
H	30.122500	4.217800	16.592500
H	29.110000	5.065500	15.394400
H	29.043900	3.279700	15.495200
C	30.310000	3.849400	13.242900
H	30.981800	4.309000	12.503700
C	30.192800	2.339800	13.007100
H	29.812000	1.876100	13.934700
H	31.203200	1.937600	12.816400
N	29.281200	1.971800	11.921800
H	29.028700	2.742600	11.275000
C	29.711400	0.813700	11.140300
H	29.857100	-0.050000	11.807000
H	28.924600	0.560400	10.416500
H	30.662500	1.001100	10.607400
H	31.397000	3.306700	14.874500
H	29.325300	4.333200	13.142500
Mg	34.197000	6.437400	5.842800
O	31.310700	8.053300	4.968900
O	33.750000	4.620000	6.770500
O	32.357200	6.930900	6.633100
O	32.580100	4.066100	2.644600
O	33.076100	5.541300	4.284200
H	29.072900	8.746600	5.503900
H	34.237900	0.099700	7.002900
H	33.102300	1.789000	3.173900
C	33.682700	3.392000	6.164300
C	29.028300	8.466800	6.557500
C	33.972000	0.951900	6.370000
C	33.962200	2.229200	6.938300
C	31.331200	7.604500	6.177200
C	33.360000	3.196800	4.768300
C	33.370100	1.884600	4.227500
C	32.980700	4.311100	3.845000
Mg	32.561100	5.495400	8.196000
Mg	34.197600	6.437100	12.862300
Mg	32.569400	7.387800	10.519600
O	31.217500	6.788600	9.097900
O	33.912900	6.852000	8.987000
O	31.311300	8.053000	11.988400
O	33.750500	4.619700	13.790000
O	32.357800	6.930500	13.652600
O	32.580600	4.065800	9.664100
O	34.358000	7.918100	11.447400
O	33.076600	5.541000	11.303700
O	35.399500	7.199100	7.316700
H	29.073400	8.746300	12.523400
H	34.181500	2.365100	8.001000
H	34.238400	0.099400	14.022400
H	33.102900	1.788600	10.193400

H	38.031800	10.595000	11.686300
H	36.093000	9.414400	12.680100
H	37.131400	8.785500	7.849200
H	27.059100	8.618700	9.342800
H	29.057300	7.535300	10.336900
C	33.683300	3.391600	13.183800
C	30.174400	7.829700	7.097600
C	29.028800	8.466400	13.577000
C	33.972600	0.951600	13.389500
C	33.962800	2.228800	13.957800
C	31.331800	7.604200	13.196700
C	35.453500	8.475700	10.840900
C	33.360600	3.196500	11.787800
C	33.370600	1.884300	11.247000
C	37.422800	9.944700	11.050700
C	36.321500	9.296400	11.617200
C	32.981300	4.310800	10.864500
C	30.185300	7.456800	8.494200
C	35.781800	8.299300	9.443200
C	36.912400	8.967300	8.902700
C	37.746500	9.802700	9.667900
C	27.927800	8.417200	8.708500
C	29.042100	7.792400	9.274200
C	35.005500	7.408100	8.525500
Mg	32.570000	7.387500	17.539100
O	31.218100	6.788200	16.117400
O	33.862400	6.902700	16.002900
O	33.751100	4.619300	20.809500
O	32.581200	4.065400	16.683600
O	34.358600	7.917800	18.466900
O	33.077200	5.540600	18.323200
O	35.400000	7.198800	14.336200
H	34.182000	2.364800	15.020400
H	34.239000	0.099100	21.041900
H	33.103400	1.788300	17.212900
H	38.032400	10.594700	18.705700
H	36.093500	9.414100	19.699600
H	37.132000	8.785200	14.868700
H	27.059700	8.618400	16.362300
H	29.057900	7.535000	17.356400
C	33.683800	3.391300	20.203300
C	30.175000	7.829400	14.117100
C	33.973100	0.951300	20.409000
C	33.963300	2.228500	20.977300
C	35.454100	8.475400	17.860400
C	33.361100	3.196200	18.807300
C	33.371200	1.884000	18.266500
C	37.423300	9.944400	18.070200
C	36.322100	9.296100	18.636700
C	32.981900	4.310500	17.884000
C	30.185800	7.456400	15.513700
C	35.782400	8.299000	16.462700
C	36.913000	8.967000	15.922200
C	37.747000	9.802400	16.687300
C	27.928400	8.416800	15.728000
C	29.042600	7.792000	16.293700
C	35.006100	7.407800	15.545000
H	38.612600	10.315200	16.242000
H	38.612000	10.314700	9.222400
H	33.601400	5.288800	20.060300
H	32.413200	3.096700	2.517700
H	34.215300	2.370900	22.039900
Mg	32.561700	5.495100	15.215500
C	33.679000	0.743400	4.989000
H	33.690500	-0.229000	4.542700
C	33.679600	0.743100	12.008500
H	33.691100	-0.229300	11.562200
C	33.680100	0.742800	19.028000
H	33.691600	-0.229600	18.581700
C	27.890300	8.765100	14.345400
H	27.037700	9.234000	13.900300
C	27.889700	8.765400	7.325900
H	27.037000	9.234100	6.880800

==========

TS_1(C-axis)

==========

145

ENERGY = -5387.617136201

C	27.747600	1.778700	12.524900
O	26.939500	1.451000	11.616300
O	27.609200	2.041700	13.719200
N	30.786000	4.215000	7.532000
C	29.784900	4.278900	8.606900

H	30.325600	4.291500	9.562800
C	28.754300	3.151800	8.646900
H	29.244900	2.170000	8.550100
H	28.002600	3.249900	7.845700
N	28.083900	3.173700	9.964900
H	27.414600	2.380200	10.123300
C	27.387100	4.432500	10.312300
H	26.680200	4.711500	9.516200
H	26.839700	4.258200	11.247500
H	28.112400	5.244500	10.448800
H	29.271700	5.243800	8.513000
H	31.232600	3.291500	7.553300
C	30.213800	4.458600	6.194600
H	31.026100	4.627800	5.479000
H	29.567000	3.635100	5.842100
H	29.622700	5.383700	6.234300
N	30.818900	4.121400	14.598000
C	29.706800	4.143400	15.582600
H	30.134000	4.161800	16.592100
H	29.122600	5.061000	15.430100
H	29.035900	3.276500	15.459500
C	30.284400	3.858600	13.237900
H	30.933200	4.342100	12.491500
C	30.191800	2.347500	12.987800
H	29.899700	1.861500	13.934900
H	31.185000	1.977000	12.694600
N	29.217000	1.954100	11.954800
H	28.809900	2.831400	10.853200
C	29.654900	0.729700	11.253200
H	29.818100	-0.100400	11.962700
H	28.873500	0.428400	10.543700
H	30.601300	0.925500	10.723800
H	31.394200	3.306300	14.847900
H	29.285000	4.314600	13.169700
Mg	34.197000	6.437400	5.842800
O	31.310700	8.053300	4.968900
O	33.750000	4.620000	6.770500
O	32.357200	6.930900	6.633100
O	32.580100	4.066100	2.644600
O	33.076100	5.541300	4.284200
H	29.072900	8.746600	5.503900
H	34.237900	0.099700	7.002900
H	33.102300	1.789000	3.173900
C	33.682700	3.392000	6.164300
C	29.028300	8.466800	6.557500
C	33.972000	0.951900	6.370000
C	33.962200	2.229200	6.938300
C	31.331200	7.604500	6.177200
C	33.360000	3.196800	4.768300
C	33.370100	1.884600	4.227500
C	32.980700	4.311100	3.845000
Mg	32.561100	5.495400	8.196000
Mg	34.197600	6.437100	12.862300
Mg	32.569400	7.387800	10.519600
O	31.217500	6.788600	9.097900
O	33.912900	6.852000	8.987000
O	31.311300	8.053000	11.988400
O	33.750500	4.619700	13.790000
O	32.357800	6.930500	13.652600
O	32.580600	4.065800	9.664100
O	34.358000	7.918100	11.447400
O	33.076600	5.541000	11.303700
O	35.399500	7.199100	7.316700
H	29.073400	8.746300	12.523400
H	34.181500	2.365100	8.001000
H	34.238400	0.099400	14.022400
H	33.102900	1.788600	10.193400
H	38.031800	10.595000	11.686300
H	36.093000	9.414400	12.680100
H	37.131400	8.785500	7.849200
H	27.059100	8.618700	9.342800
H	29.057300	7.535300	10.336900
C	33.683300	3.391600	13.183800
C	30.174400	7.829700	7.097600
C	29.028800	8.466400	13.577000
C	33.972600	0.951600	13.389500
C	33.962800	2.228800	13.957800
C	31.331800	7.604200	13.196700
C	35.453500	8.475700	10.840900
C	33.360600	3.196500	11.787800
C	33.370600	1.884300	11.247000
C	37.422800	9.944700	11.050700
C	36.321500	9.296400	11.617200
C	32.981300	4.310800	10.864500

C	30.185300	7.456800	8.494200
C	35.781800	8.299300	9.443200
C	36.912400	8.967300	8.902700
C	37.746500	9.802700	9.667900
C	27.927800	8.417200	8.708500
C	29.042100	7.792400	9.274200
C	35.005500	7.408100	8.525500
Mg	32.570000	7.387500	17.539100
O	31.218100	6.788200	16.117400
O	33.862400	6.902700	16.002900
O	33.751100	4.619300	20.809500
O	32.581200	4.065400	16.683600
O	34.358600	7.917800	18.466900
O	33.077200	5.540600	18.323200
O	35.400000	7.198800	14.336200
H	34.182000	2.364800	15.020400
H	34.239000	0.099100	21.041900
H	33.103400	1.788300	17.212900
H	38.032400	10.594700	18.705700
H	36.093500	9.414100	19.699600
H	37.132000	8.785200	14.868700
H	27.059700	8.618400	16.362300
H	29.057900	7.535000	17.356400
C	33.683800	3.391300	20.203300
C	30.175000	7.829400	14.117100
C	33.973100	0.951300	20.409000
C	33.963300	2.228500	20.977300
C	35.454100	8.475400	17.860400
C	33.361100	3.196200	18.807300
C	33.371200	1.884000	18.266500
C	37.423300	9.944400	18.070200
C	36.322100	9.296100	18.636700
C	32.981900	4.310500	17.884000
C	30.185800	7.456400	15.513700
C	35.782400	8.299000	16.462700
C	36.913000	8.967000	15.922200
C	37.747000	9.802400	16.687300
C	27.928400	8.416800	15.728000
C	29.042600	7.792000	16.293700
C	35.006100	7.407800	15.545000
H	38.612600	10.315200	16.242000
H	38.612000	10.314700	9.222400
H	33.601400	5.288800	20.060300
H	32.413200	3.096700	2.517700
H	34.215300	2.370900	22.039900
Mg	32.561700	5.495100	15.215500
C	33.679000	0.743400	4.989000
H	33.690500	-0.229000	4.542700
C	33.679600	0.743100	12.008500
H	33.691100	-0.229300	11.562200
C	33.680100	0.742800	19.028000
H	33.691600	-0.229600	18.581700
C	27.890300	8.765100	14.345400
H	27.037700	9.234000	13.900300
C	27.889700	8.765400	7.325900
H	27.037000	9.234100	6.880800

==========

TS_2(C-axis)

==========

145

ENERGY = -5387.629831699

C	27.942700	1.704000	12.277200
O	27.141100	1.366400	11.240300
O	27.526200	1.812300	13.422800
N	30.786400	4.266300	7.447000
C	29.735200	4.294500	8.476700
H	30.234100	4.205700	9.454000
C	28.649200	3.223600	8.384800
H	29.108900	2.221700	8.352300
H	28.038600	3.339300	7.476500
N	27.762300	3.319300	9.560200
H	27.355700	1.971400	10.432000
C	26.653600	4.275000	9.387100
H	25.976000	3.900900	8.606100
H	26.090500	4.336400	10.328900
H	26.995500	5.288700	9.105900
H	29.264700	5.285500	8.444500
H	31.209300	3.331000	7.447300
C	30.253200	4.556100	6.100400
H	31.074600	4.823700	5.428700
H	29.673400	3.716400	5.678400
H	29.599000	5.436000	6.169600
N	30.830000	4.119600	14.621700

C	29.703200	4.175600	15.583200
H	30.111300	4.229300	16.599200
H	29.119400	5.085000	15.388400
H	29.034000	3.302400	15.488700
C	30.324200	3.842400	13.257300
H	31.011500	4.274200	12.516200
C	30.166500	2.326700	13.054500
H	29.753800	1.898000	13.980600
H	31.159400	1.884900	12.875700
N	29.285300	1.955000	11.946500
H	28.338900	3.640900	10.348900
C	29.946700	1.328600	10.803100
H	29.198000	0.923300	10.114800
H	30.578300	2.058600	10.270100
H	30.599800	0.504300	11.141000
H	31.398300	3.308500	14.899700
H	29.348100	4.337700	13.143700
Mg	34.197000	6.437400	5.842800
O	31.310700	8.053300	4.968900
O	33.750000	4.620000	6.770500
O	32.357200	6.930900	6.633100
O	32.580100	4.066100	2.644600
O	33.076100	5.541300	4.284200
H	29.072900	8.746600	5.503900
H	34.237900	0.099700	7.002900
H	33.102300	1.789000	3.173900
C	33.682700	3.392000	6.164300
C	29.028300	8.466800	6.557500
C	33.972000	0.951900	6.370000
C	33.962200	2.229200	6.938300
C	31.331200	7.604500	6.177200
C	33.360000	3.196800	4.768300
C	33.370100	1.884600	4.227500
C	32.980700	4.311100	3.845000
Mg	32.561100	5.495400	8.196000
Mg	34.197600	6.437100	12.862300
Mg	32.569400	7.387800	10.519600
O	31.217500	6.788600	9.097900
O	33.912900	6.852000	8.987000
O	31.311300	8.053000	11.988400
O	33.750500	4.619700	13.790000
O	32.357800	6.930500	13.652600
O	32.580600	4.065800	9.664100
O	34.358000	7.918100	11.447400
O	33.076600	5.541000	11.303700
O	35.399500	7.199100	7.316700
H	29.073400	8.746300	12.523400
H	34.181500	2.365100	8.001000
H	34.238400	0.099400	14.022400
H	33.102900	1.788600	10.193400
H	38.031800	10.595000	11.686300
H	36.093000	9.414400	12.680100
H	37.131400	8.785500	7.849200
H	27.059100	8.618700	9.342800
H	29.057300	7.535300	10.336900
C	33.683300	3.391600	13.183800
C	30.174400	7.829700	7.097600
C	29.028800	8.466400	13.577000
C	33.972600	0.951600	13.389500
C	33.962800	2.228800	13.957800
C	31.331800	7.604200	13.196700
C	35.453500	8.475700	10.840900
C	33.360600	3.196500	11.787800
C	33.370600	1.884300	11.247000
C	37.422800	9.944700	11.050700
C	36.321500	9.296400	11.617200
C	32.981300	4.310800	10.864500
C	30.185300	7.456800	8.494200
C	35.781800	8.299300	9.443200
C	36.912400	8.967300	8.902700
C	37.746500	9.802700	9.667900
C	27.927800	8.417200	8.708500
C	29.042100	7.792400	9.274200
C	35.005500	7.408100	8.525500
Mg	32.570000	7.387500	17.539100
O	31.218100	6.788200	16.117400
O	33.862400	6.902700	16.002900
O	33.751100	4.619300	20.809500
O	32.581200	4.065400	16.683600
O	34.358600	7.917800	18.466900
O	33.077200	5.540600	18.323200
O	35.400000	7.198800	14.336200
H	34.182000	2.364800	15.020400
H	34.239000	0.099100	21.041900

H	33.103400	1.788300	17.212900
H	38.032400	10.594700	18.705700
H	36.093500	9.414100	19.699600
H	37.132000	8.785200	14.868700
H	27.059700	8.618400	16.362300
H	29.057900	7.535000	17.356400
C	33.683800	3.391300	20.203300
C	30.175000	7.829400	14.117100
C	33.973100	0.951300	20.409000
C	33.963300	2.228500	20.977300
C	35.454100	8.475400	17.860400
C	33.361100	3.196200	18.807300
C	33.371200	1.884000	18.266500
C	37.423300	9.944400	18.070200
C	36.322100	9.296100	18.636700
C	32.981900	4.310500	17.884000
C	30.185800	7.456400	15.513700
C	35.782400	8.299000	16.462700
C	36.913000	8.967000	15.922200
C	37.747000	9.802400	16.687300
C	27.928400	8.416800	15.728000
C	29.042600	7.792000	16.293700
C	35.006100	7.407800	15.545000
H	38.612600	10.315200	16.242000
H	38.612000	10.314700	9.222400
H	33.601400	5.288800	20.060300
H	32.413200	3.096700	2.517700
H	34.215300	2.370900	22.039900
Mg	32.561700	5.495100	15.215500
C	33.679000	0.743400	4.989000
H	33.690500	-0.229000	4.542700
C	33.679600	0.743100	12.008500
H	33.691100	-0.229300	11.562200
C	33.680100	0.742800	19.028000
H	33.691600	-0.229600	18.581700
C	27.890300	8.765100	14.345400
H	27.037700	9.234000	13.900300
C	27.889700	8.765400	7.325900
H	27.037000	9.234100	6.880800

==========

B_I(C-axis)

==========

145

ENERGY = -5387.629996730

C	27.972104	1.603200	12.337799
O	27.174564	1.258819	11.298631
O	27.549536	1.710206	13.481141
N	30.799572	4.254302	7.444460
C	29.751386	4.260241	8.477917
H	30.256621	4.206867	9.454500
C	28.715692	3.137623	8.409233
H	29.227297	2.160421	8.376755
H	28.087249	3.213793	7.508254
N	27.840526	3.189027	9.594181
H	27.410578	1.835329	10.480190
C	26.722725	4.140438	9.458528
H	26.045947	3.785601	8.667939
H	26.163398	4.163787	10.404211
H	27.052188	5.166207	9.209590
H	29.244900	5.233437	8.431029
H	31.236483	3.325491	7.439014
C	30.258528	4.541294	6.100548
H	31.076767	4.806503	5.423862
H	29.675967	3.701157	5.683604
H	29.606028	5.422118	6.171752
N	30.825738	4.106748	14.637510
C	29.697851	4.181069	15.596460
H	30.104585	4.263843	16.610811
H	29.108390	5.081870	15.377860
H	29.034363	3.301006	15.524651
C	30.323263	3.789325	13.280885
H	31.003835	4.211709	12.528450
C	30.185854	2.266850	13.113615
H	29.774442	1.854322	14.047353
H	31.184248	1.833081	12.947828
N	29.312774	1.861670	12.011380
H	28.422317	3.492969	10.386132
C	29.984557	1.253599	10.864995
H	29.244542	0.824848	10.181104
H	30.590001	2.000870	10.325058
H	30.665115	0.451237	11.200265
H	31.398115	3.306641	14.938741

H	29.339820	4.267217	13.155996
Mg	34.197009	6.437400	5.842800
O	31.310706	8.053303	4.968900
O	33.750009	4.620000	6.770503
O	32.357206	6.930903	6.633103
O	32.580109	4.066100	2.644600
O	33.076109	5.541300	4.284200
H	29.072906	8.746603	5.503900
H	34.237909	0.099700	7.002903
H	33.102309	1.789000	3.173900
C	33.682709	3.392000	6.164300
C	29.028306	8.466803	6.557503
C	33.972009	0.951900	6.370000
C	33.962209	2.229200	6.938303
C	31.331206	7.604503	6.177200
C	33.360009	3.196800	4.768300
C	33.370109	1.884600	4.227500
C	32.980709	4.311100	3.845000
Mg	32.561109	5.495400	8.196003
Mg	34.197609	6.437100	12.862303
Mg	32.569409	7.387803	10.519603
O	31.217506	6.788603	9.097903
O	33.912909	6.852003	8.987003
O	31.311306	8.053003	11.988403
O	33.750509	4.619700	13.790003
O	32.357806	6.930503	13.652603
O	32.580609	4.065800	9.664103
O	34.358009	7.918103	11.447403
O	33.076609	5.541000	11.303703
O	35.399509	7.199103	7.316703
H	29.073406	8.746303	12.523403
H	34.181509	2.365100	8.001003
H	34.238409	0.099400	14.022403
H	33.102909	1.788600	10.193403
H	38.031809	10.595003	11.686303
H	36.093009	9.414403	12.680103
H	37.131409	8.785503	7.849203
H	27.059106	8.618703	9.342803
H	29.057306	7.535303	10.336903
C	33.683309	3.391600	13.183803
C	30.174406	7.829703	7.097603
C	29.028806	8.466403	13.577003
C	33.972609	0.951600	13.389503
C	33.962809	2.228800	13.957803
C	31.331806	7.604203	13.196703
C	35.453509	8.475703	10.840903
C	33.360609	3.196500	11.787803
C	33.370609	1.884300	11.247003
C	37.422809	9.944703	11.050703
C	36.321509	9.296403	11.617203
C	32.981309	4.310800	10.864503
C	30.185306	7.456803	8.494203
C	35.781809	8.299303	9.443203
C	36.912409	8.967303	8.902703
C	37.746509	9.802703	9.667903
C	27.927806	8.417203	8.708503
C	29.042106	7.792403	9.274203
C	35.005509	7.408103	8.525503
Mg	32.570009	7.387503	17.539103
O	31.218106	6.788203	16.117403
O	33.862409	6.902703	16.002903
O	33.751109	4.619300	20.809506
O	32.581209	4.065400	16.683603
O	34.358609	7.917803	18.466903
O	33.077209	5.540600	18.323203
O	35.400009	7.198803	14.336203
H	34.182009	2.364800	15.020403
H	34.239009	0.099100	21.041906
H	33.103409	1.788300	17.212903
H	38.032409	10.594703	18.705703
H	36.093509	9.414103	19.699606
H	37.132009	8.785203	14.868703
H	27.059706	8.618403	16.362303
H	29.057906	7.535003	17.356403
C	33.683809	3.391300	20.203306
C	30.175006	7.829403	14.117103
C	33.973109	0.951300	20.409006
C	33.963309	2.228500	20.977306
C	35.454109	8.475403	17.860403
C	33.361109	3.196200	18.807303
C	33.371209	1.884000	18.266503
C	37.423309	9.944403	18.070203
C	36.322109	9.296103	18.636703
C	32.981909	4.310500	17.884003

C	30.185806	7.456403	15.513703
C	35.782409	8.299003	16.462703
C	36.913009	8.967003	15.922203
C	37.747009	9.802403	16.687303
C	27.928406	8.416803	15.728003
C	29.042606	7.792003	16.293703
C	35.006109	7.407803	15.545003
H	38.612609	10.315203	16.242003
H	38.612009	10.314703	9.222403
H	33.601409	5.288800	20.060306
H	32.413206	3.096700	2.517700
H	34.215309	2.370900	22.039906
Mg	32.561709	5.495100	15.215503
C	33.679009	0.743400	4.989000
H	33.690509	-0.229000	4.542700
C	33.679609	0.743100	12.008503
H	33.691109	-0.229300	11.562203
C	33.680109	0.742800	19.028003
H	33.691609	-0.229600	18.581703
C	27.890306	8.765103	14.345403
H	27.037706	9.234003	13.900303
C	27.889706	8.765403	7.325903
H	27.037006	9.234103	6.880803

==========

B_{II}(C-axis)

==========

145

ENERGY = -5387.635331390

C	28.250075	2.041178	11.541301
O	27.892777	1.272809	10.485187
O	27.708764	3.120040	11.821113
N	30.796264	4.273879	7.436808
C	29.656242	4.271788	8.379188
H	30.059619	4.203807	9.400495
C	28.644020	3.149380	8.136906
H	29.100229	2.181750	8.411967
H	28.375813	3.094746	7.070440
N	27.396165	3.324415	8.904873
H	27.390744	1.899260	9.843797
C	26.371591	4.092503	8.188070
H	26.019209	3.515914	7.319240
H	25.518852	4.261464	8.860438
H	26.738030	5.075282	7.831099
H	29.155481	5.246008	8.289818
H	31.228091	3.342713	7.463811
C	30.355806	4.561331	6.055190
H	31.204306	4.916408	5.466061
H	29.884051	3.694996	5.560110
H	29.629739	5.385567	6.088738
N	30.762730	4.035021	14.731607
C	29.658355	4.290346	15.684786
H	30.083027	4.660479	16.624453
H	29.003164	5.067588	15.267404
H	29.050910	3.393415	15.893046
C	30.260671	3.558912	13.428563
H	31.102817	3.485351	12.729425
C	29.585493	2.178949	13.548380
H	28.653334	2.271168	14.127395
H	30.265622	1.507462	14.096628
N	29.285573	1.532688	12.273180
H	27.598099	3.806299	9.792252
C	29.949884	0.270412	11.976552
H	29.713338	-0.030745	10.950737
H	31.038552	0.399089	12.079367
H	29.617557	-0.527864	12.665277
H	31.327551	3.279886	15.139351
H	29.540751	4.287195	13.031958
Mg	34.197003	6.437400	5.842800
O	31.310702	8.053301	4.968900
O	33.750003	4.620000	6.770501
O	32.357202	6.930901	6.633101
O	32.580103	4.066100	2.644600
O	33.076103	5.541300	4.284200
H	29.072902	8.746601	5.503900
H	34.237903	0.099700	7.002901
H	33.102303	1.789000	3.173900
C	33.682703	3.392000	6.164300
C	29.028302	8.466801	6.557501
C	33.972003	0.951900	6.370000
C	33.962203	2.229200	6.938301
C	31.331202	7.604501	6.177200
C	33.360003	3.196800	4.768300
C	33.370103	1.884600	4.227500

C	32.980703	4.311100	3.845000
Mg	32.561103	5.495400	8.196001
Mg	34.197603	6.437100	12.862301
Mg	32.569403	7.387801	10.519601
O	31.217502	6.788601	9.097901
O	33.912903	6.852001	8.987001
O	31.311302	8.053001	11.988401
O	33.750503	4.619700	13.790001
O	32.357802	6.930501	13.652601
O	32.580603	4.065800	9.664101
O	34.358003	7.918101	11.447401
O	33.076603	5.541000	11.303701
O	35.399503	7.199101	7.316701
H	29.073402	8.746301	12.523401
H	34.181503	2.365100	8.001001
H	34.238403	0.099400	14.022401
H	33.102903	1.788600	10.193401
H	38.031803	10.595001	11.686301
H	36.093003	9.414401	12.680101
H	37.131403	8.785501	7.849201
H	27.059102	8.618701	9.342801
H	29.057302	7.535301	10.336901
C	33.683303	3.391600	13.183801
C	30.174402	7.829701	7.097601
C	29.028802	8.466401	13.577001
C	33.972603	0.951600	13.389501
C	33.962803	2.228800	13.957801
C	31.331802	7.604201	13.196701
C	35.453503	8.475701	10.840901
C	33.360603	3.196500	11.787801
C	33.370603	1.884300	11.247001
C	37.422803	9.944701	11.050701
C	36.321503	9.296401	11.617201
C	32.981303	4.310800	10.864501
C	30.185302	7.456801	8.494201
C	35.781803	8.299301	9.443201
C	36.912403	8.967301	8.902701
C	37.746503	9.802701	9.667901
C	27.927802	8.417201	8.708501
C	29.042102	7.792401	9.274201
C	35.005503	7.408101	8.525501
Mg	32.570003	7.387501	17.539101
O	31.218102	6.788201	16.117401
O	33.862403	6.902701	16.002901
O	33.751103	4.619300	20.809502
O	32.581203	4.065400	16.683601
O	34.358603	7.917801	18.466901
O	33.077203	5.540600	18.323201
O	35.400003	7.198801	14.336201
H	34.182003	2.364800	15.020401
H	34.239003	0.099100	21.041902
H	33.103403	1.788300	17.212901
H	38.032403	10.594701	18.705701
H	36.093503	9.414101	19.699602
H	37.132003	8.785201	14.868701
H	27.059702	8.618401	16.362301
H	29.057902	7.535001	17.356401
C	33.683803	3.391300	20.203302
C	30.175002	7.829401	14.117101
C	33.973103	0.951300	20.409002
C	33.963303	2.228500	20.977302
C	35.454103	8.475401	17.860401
C	33.361103	3.196200	18.807301
C	33.371203	1.884000	18.266501
C	37.423303	9.944401	18.070201
C	36.322103	9.296101	18.636701
C	32.981903	4.310500	17.884001
C	30.185802	7.456401	15.513701
C	35.782403	8.299001	16.462701
C	36.913003	8.967001	15.922201
C	37.747003	9.802401	16.687301
C	27.928402	8.416801	15.728001
C	29.042602	7.792001	16.293701
C	35.006103	7.407801	15.545001
H	38.612603	10.315201	16.242001
H	38.612003	10.314701	9.222401
H	33.601403	5.288800	20.060302
H	32.413202	3.096700	2.517700
H	34.215303	2.370900	22.039902
Mg	32.561703	5.495100	15.215501
C	33.679003	0.743400	4.989000
H	33.690503	-0.229000	4.542700
C	33.679603	0.743100	12.008501
H	33.691103	-0.229300	11.562201

C	33.680103	0.742800	19.028001
H	33.691603	-0.229600	18.581701
C	27.890302	8.765101	14.345401
H	27.037702	9.234001	13.900301
C	27.889702	8.765401	7.325901
H	27.037002	9.234101	6.880801

==========

B_{III}(C-axis)

==========

148

ENERGY = -5576.106146861

C	26.454613	-0.093328	6.314389
O	26.631247	0.706225	7.152869
O	26.279945	-0.889401	5.472387
C	28.461799	2.174943	11.393255
O	27.977844	1.385425	10.408000
O	27.971205	3.273256	11.687514
N	30.788123	4.267140	7.425010
C	29.632755	4.261663	8.350461
H	30.015706	4.103986	9.369681
C	28.565664	3.218468	8.014981
H	28.977405	2.204766	8.167517
H	28.274858	3.297228	6.956450
N	27.349046	3.376783	8.841583
H	27.440555	2.017924	9.784881
C	26.220371	3.981944	8.131524
H	25.869339	3.294436	7.348209
H	25.397030	4.145637	8.841866
H	26.478485	4.952384	7.662693
H	29.183319	5.264034	8.319968
H	31.213419	3.333073	7.449520
C	30.369443	4.571455	6.040214
H	31.225086	4.943858	5.471506
H	29.914207	3.709236	5.524518
H	29.634802	5.388397	6.073240
N	30.807746	4.092559	14.675891
C	29.680313	4.261872	15.618009
H	30.084095	4.481360	16.613469
H	29.069670	5.114396	15.292279
H	29.032953	3.369389	15.675358
C	30.335350	3.731367	13.321904
H	31.113066	3.964475	12.586669
C	30.012058	2.228732	13.285762
H	29.260224	2.005654	14.065612
H	30.939735	1.697389	13.552785
N	29.578768	1.661221	12.006978
H	27.564046	3.941070	9.673917
C	30.024431	0.294151	11.749769
H	29.767295	0.011148	10.724395
H	31.115363	0.251412	11.883806
H	29.550645	-0.425566	12.443373
H	31.369886	3.309141	15.033379
H	29.448740	4.327376	13.080424
Mg	34.197003	6.437400	5.842800
O	31.310702	8.053301	4.968900
O	33.750003	4.620000	6.770501
O	32.357202	6.930901	6.633101
O	32.580103	4.066100	2.644600
O	33.076103	5.541300	4.284200
H	29.072902	8.746601	5.503900
H	34.237903	0.099700	7.002901
H	33.102303	1.789000	3.173900
C	33.682703	3.392000	6.164300
C	29.028302	8.466801	6.557501
C	33.972003	0.951900	6.370000
C	33.962203	2.229200	6.938301
C	31.331202	7.604501	6.177200
C	33.360003	3.196800	4.768300
C	33.370103	1.884600	4.227500
C	32.980703	4.311100	3.845000
Mg	32.561103	5.495400	8.196001
Mg	34.197603	6.437100	12.862301
Mg	32.569403	7.387801	10.519601
O	31.217502	6.788601	9.097901
O	33.912903	6.852001	8.987001
O	31.311302	8.053001	11.988401
O	33.750503	4.619700	13.790001
O	32.357802	6.930501	13.652601
O	32.580603	4.065800	9.664101
O	34.358003	7.918101	11.447401
O	33.076603	5.541000	11.303701
O	35.399503	7.199101	7.316701
H	29.073402	8.746301	12.523401

H	34.181503	2.365100	8.001001
H	34.238403	0.099400	14.022401
H	33.102903	1.788600	10.193401
H	38.031803	10.595001	11.686301
H	36.093003	9.414401	12.680101
H	37.131403	8.785501	7.849201
H	27.059102	8.618701	9.342801
H	29.057302	7.535301	10.336901
C	33.683303	3.391600	13.183801
C	30.174402	7.829701	7.097601
C	29.028802	8.466401	13.577001
C	33.972603	0.951600	13.389501
C	33.962803	2.228800	13.957801
C	31.331802	7.604201	13.196701
C	35.453503	8.475701	10.840901
C	33.360603	3.196500	11.787801
C	33.370603	1.884300	11.247001
C	37.422803	9.944701	11.050701
C	36.321503	9.296401	11.617201
C	32.981303	4.310800	10.864501
C	30.185302	7.456801	8.494201
C	35.781803	8.299301	9.443201
C	36.912403	8.967301	8.902701
C	37.746503	9.802701	9.667901
C	27.927802	8.417201	8.708501
C	29.042102	7.792401	9.274201
C	35.005503	7.408101	8.525501
Mg	32.570003	7.387501	17.539101
O	31.218102	6.788201	16.117401
O	33.862403	6.902701	16.002901
O	33.751103	4.619300	20.809502
O	32.581203	4.065400	16.683601
O	34.358603	7.917801	18.466901
O	33.077203	5.540600	18.323201
O	35.400003	7.198801	14.336201
H	34.182003	2.364800	15.020401
H	34.239003	0.099100	21.041902
H	33.103403	1.788300	17.212901
H	38.032403	10.594701	18.705701
H	36.093503	9.414101	19.699602
H	37.132003	8.785201	14.868701
H	27.059702	8.618401	16.362301
H	29.057902	7.535001	17.356401
C	33.683803	3.391300	20.203302
C	30.175002	7.829401	14.117101
C	33.973103	0.951300	20.409002
C	33.963303	2.228500	20.977302
C	35.454103	8.475401	17.860401
C	33.361103	3.196200	18.807301
C	33.371203	1.884000	18.266501
C	37.423303	9.944401	18.070201
C	36.322103	9.296101	18.636701
C	32.981903	4.310500	17.884001
C	30.185802	7.456401	15.513701
C	35.782403	8.299001	16.462701
C	36.913003	8.967001	15.922201
C	37.747003	9.802401	16.687301
C	27.928402	8.416801	15.728001
C	29.042602	7.792001	16.293701
C	35.006103	7.407801	15.545001
H	38.612603	10.315201	16.242001
H	38.612003	10.314701	9.222401
H	33.601403	5.288800	20.060302
H	32.413202	3.096700	2.517700
H	34.215303	2.370900	22.039902
Mg	32.561703	5.495100	15.215501
C	33.679003	0.743400	4.989000
H	33.690503	-0.229000	4.542700
C	33.679603	0.743100	12.008501
H	33.691103	-0.229300	11.562201
C	33.680103	0.742800	19.028001
H	33.691603	-0.229600	18.581701
C	27.890302	8.765101	14.345401
H	27.037702	9.234001	13.900301
C	27.889702	8.765401	7.325901
H	27.037002	9.234101	6.880801

==========

ZW_2(C-axis)

==========

148

ENERGY = -5576.119401011

C	26.182804	2.200566	8.809505
O	25.521717	2.299702	9.847007

O	26.311881	1.484807	7.841552
C	27.966556	2.636659	12.044323
O	26.839239	1.917032	12.148738
O	28.087339	3.640764	11.311872
N	30.780690	4.242728	7.423319
C	29.638632	4.240583	8.361459
H	30.018226	4.027261	9.369838
C	28.515210	3.261909	7.994035
H	28.799423	2.224219	8.222742
H	28.267864	3.303130	6.924271
N	27.273886	3.560195	8.744313
H	26.239734	2.172852	11.378962
C	26.534983	4.737706	8.239645
H	26.221684	4.541459	7.204436
H	25.650290	4.877055	8.873825
H	27.156416	5.645529	8.275624
H	29.243777	5.264207	8.379476
H	31.208669	3.310214	7.429838
C	30.360522	4.574590	6.044240
H	31.217225	4.953350	5.482122
H	29.902694	3.723207	5.512707
H	29.629382	5.393477	6.092126
N	30.845421	4.178468	14.587895
C	29.681173	4.171548	15.493496
H	30.048194	4.146814	16.527556
H	29.110643	5.097904	15.346550
H	29.008299	3.314597	15.315449
C	30.490249	4.211117	13.156298
H	31.290331	4.736829	12.623264
C	30.306371	2.830102	12.527052
H	31.088654	2.147693	12.894158
H	30.438645	2.917779	11.437320
N	29.010423	2.197838	12.795433
H	27.512827	3.703622	9.757781
C	28.975321	1.003017	13.628866
H	27.951374	0.619698	13.680086
H	29.634385	0.223373	13.210459
H	29.320959	1.242561	14.648108
H	31.379058	3.319867	14.768300
H	29.576453	4.805440	13.024050
Mg	34.197003	6.437400	5.842800
O	31.310702	8.053301	4.968900
O	33.750003	4.620000	6.770501
O	32.357202	6.930901	6.633101
O	32.580103	4.066100	2.644600
O	33.076103	5.541300	4.284200
H	29.072902	8.746601	5.503900
H	34.237903	0.099700	7.002901
H	33.102303	1.789000	3.173900
C	33.682703	3.392000	6.164300
C	29.028302	8.466801	6.557501
C	33.972003	0.951900	6.370000
C	33.962203	2.229200	6.938301
C	31.331202	7.604501	6.177200
C	33.360003	3.196800	4.768300
C	33.370103	1.884600	4.227500
C	32.980703	4.311100	3.845000
Mg	32.561103	5.495400	8.196001
Mg	34.197603	6.437100	12.862301
Mg	32.569403	7.387801	10.519601
O	31.217502	6.788601	9.097901
O	33.912903	6.852001	8.987001
O	31.311302	8.053001	11.988401
O	33.750503	4.619700	13.790001
O	32.357802	6.930501	13.652601
O	32.580603	4.065800	9.664101
O	34.358003	7.918101	11.447401
O	33.076603	5.541000	11.303701
O	35.399503	7.199101	7.316701
H	29.073402	8.746301	12.523401
H	34.181503	2.365100	8.001001
H	34.238403	0.099400	14.022401
H	33.102903	1.788600	10.193401
H	38.031803	10.595001	11.686301
H	36.093003	9.414401	12.680101
H	37.131403	8.785501	7.849201
H	27.059102	8.618701	9.342801
H	29.057302	7.535301	10.336901
C	33.683303	3.391600	13.183801
C	30.174402	7.829701	7.097601
C	29.028802	8.466401	13.577001
C	33.972603	0.951600	13.389501
C	33.962803	2.228800	13.957801
C	31.331802	7.604201	13.196701

C	35.453503	8.475701	10.840901
C	33.360603	3.196500	11.787801
C	33.370603	1.884300	11.247001
C	37.422803	9.944701	11.050701
C	36.321503	9.296401	11.617201
C	32.981303	4.310800	10.864501
C	30.185302	7.456801	8.494201
C	35.781803	8.299301	9.443201
C	36.912403	8.967301	8.902701
C	37.746503	9.802701	9.667901
C	27.927802	8.417201	8.708501
C	29.042102	7.792401	9.274201
C	35.005503	7.408101	8.525501
Mg	32.570003	7.387501	17.539101
O	31.218102	6.788201	16.117401
O	33.862403	6.902701	16.002901
O	33.751103	4.619300	20.809502
O	32.581203	4.065400	16.683601
O	34.358603	7.917801	18.466901
O	33.077203	5.540600	18.323201
O	35.400003	7.198801	14.336201
H	34.182003	2.364800	15.020401
H	34.239003	0.099100	21.041902
H	33.103403	1.788300	17.212901
H	38.032403	10.594701	18.705701
H	36.093503	9.414101	19.699602
H	37.132003	8.785201	14.868701
H	27.059702	8.618401	16.362301
H	29.057902	7.535001	17.356401
C	33.683803	3.391300	20.203302
C	30.175002	7.829401	14.117101
C	33.973103	0.951300	20.409002
C	33.963303	2.228500	20.977302
C	35.454103	8.475401	17.860401
C	33.361103	3.196200	18.807301
C	33.371203	1.884000	18.266501
C	37.423303	9.944401	18.070201
C	36.322103	9.296101	18.636701
C	32.981903	4.310500	17.884001
C	30.185802	7.456401	15.513701
C	35.782403	8.299001	16.462701
C	36.913003	8.967001	15.922201
C	37.747003	9.802401	16.687301
C	27.928402	8.416801	15.728001
C	29.042602	7.792001	16.293701
C	35.006103	7.407801	15.545001
H	38.612603	10.315201	16.242001
H	38.612003	10.314701	9.222401
H	33.601403	5.288800	20.060302
H	32.413202	3.096700	2.517700
H	34.215303	2.370900	22.039902
Mg	32.561703	5.495100	15.215501
C	33.679003	0.743400	4.989000
H	33.690503	-0.229000	4.542700
C	33.679603	0.743100	12.008501
H	33.691103	-0.229300	11.562201
C	33.680103	0.742800	19.028001
H	33.691603	-0.229600	18.581701
C	27.890302	8.765101	14.345401
H	27.037702	9.234001	13.900301
C	27.889702	8.765401	7.325901
H	27.037002	9.234101	6.880801

==========

TS_3(C-axis)

==========

148

ENERGY = -5576.104019077

C	26.401302	2.233600	8.511401
O	25.588702	2.003700	9.535701
O	26.394499	1.634038	7.455535
C	27.990302	2.555900	11.872701
O	26.877702	1.987900	11.783001
O	28.359102	3.575700	11.093001
N	30.787210	4.251333	7.374785
C	29.641525	4.207032	8.308050
H	30.016763	3.908027	9.294622
C	28.515832	3.276100	7.843447
H	28.857976	2.230555	7.846689
H	28.198710	3.512241	6.815829
N	27.327202	3.357200	8.735101
H	26.100802	2.178800	10.550401
C	26.593600	4.646814	8.578278
H	26.276781	4.779501	7.530560

H	25.715145	4.628311	9.234788
H	27.245816	5.480050	8.871206
H	29.269898	5.235152	8.399879
H	31.218469	3.320490	7.354245
C	30.371544	4.615992	6.001499
H	31.225775	5.020337	5.455353
H	29.927127	3.772510	5.446744
H	29.628081	5.422399	6.065624
N	30.835597	4.173152	14.611369
C	29.664717	4.201704	15.506967
H	30.022667	4.211638	16.544390
H	29.097727	5.123805	15.323827
H	28.989378	3.341512	15.355730
C	30.492170	4.143269	13.177657
H	31.301522	4.639592	12.631660
C	30.296515	2.734401	12.606033
H	31.000943	2.037422	13.088522
H	30.545925	2.748600	11.535936
N	28.943731	2.184123	12.767077
H	27.808402	3.470300	10.088901
C	28.737001	1.056318	13.663720
H	27.675626	0.783758	13.657853
H	29.333201	0.186433	13.338475
H	29.039336	1.324751	14.688207
H	31.366955	3.322503	14.831544
H	29.587543	4.743472	13.011479
Mg	34.197003	6.437400	5.842800
O	31.310702	8.053301	4.968900
O	33.750003	4.620000	6.770501
O	32.357202	6.930901	6.633101
O	32.580103	4.066100	2.644600
O	33.076103	5.541300	4.284200
H	29.072902	8.746601	5.503900
H	34.237903	0.099700	7.002901
H	33.102303	1.789000	3.173900
C	33.682703	3.392000	6.164300
C	29.028302	8.466801	6.557501
C	33.972003	0.951900	6.370000
C	33.962203	2.229200	6.938301
C	31.331202	7.604501	6.177200
C	33.360003	3.196800	4.768300
C	33.370103	1.884600	4.227500
C	32.980703	4.311100	3.845000
Mg	32.561103	5.495400	8.196001
Mg	34.197603	6.437100	12.862301
Mg	32.569403	7.387801	10.519601
O	31.217502	6.788601	9.097901
O	33.912903	6.852001	8.987001
O	31.311302	8.053001	11.988401
O	33.750503	4.619700	13.790001
O	32.357802	6.930501	13.652601
O	32.580603	4.065800	9.664101
O	34.358003	7.918101	11.447401
O	33.076603	5.541000	11.303701
O	35.399503	7.199101	7.316701
H	29.073402	8.746301	12.523401
H	34.181503	2.365100	8.001001
H	34.238403	0.099400	14.022401
H	33.102903	1.788600	10.193401
H	38.031803	10.595001	11.686301
H	36.093003	9.414401	12.680101
H	37.131403	8.785501	7.849201
H	27.059102	8.618701	9.342801
H	29.057302	7.535301	10.336901
C	33.683303	3.391600	13.183801
C	30.174402	7.829701	7.097601
C	29.028802	8.466401	13.577001
C	33.972603	0.951600	13.389501
C	33.962803	2.228800	13.957801
C	31.331802	7.604201	13.196701
C	35.453503	8.475701	10.840901
C	33.360603	3.196500	11.787801
C	33.370603	1.884300	11.247001
C	37.422803	9.944701	11.050701
C	36.321503	9.296401	11.617201
C	32.981303	4.310800	10.864501
C	30.185302	7.456801	8.494201
C	35.781803	8.299301	9.443201
C	36.912403	8.967301	8.902701
C	37.746503	9.802701	9.667901
C	27.927802	8.417201	8.708501
C	29.042102	7.792401	9.274201
C	35.005503	7.408101	8.525501
Mg	32.570003	7.387501	17.539101

O	31.218102	6.788201	16.117401
O	33.862403	6.902701	16.002901
O	33.751103	4.619300	20.809502
O	32.581203	4.065400	16.683601
O	34.358603	7.917801	18.466901
O	33.077203	5.540600	18.323201
O	35.400003	7.198801	14.336201
H	34.182003	2.364800	15.020401
H	34.239003	0.099100	21.041902
H	33.103403	1.788300	17.212901
H	38.032403	10.594701	18.705701
H	36.093503	9.414101	19.699602
H	37.132003	8.785201	14.868701
H	27.059702	8.618401	16.362301
H	29.057902	7.535001	17.356401
C	33.683803	3.391300	20.203302
C	30.175002	7.829401	14.117101
C	33.973103	0.951300	20.409002
C	33.963303	2.228500	20.977302
C	35.454103	8.475401	17.860401
C	33.361103	3.196200	18.807301
C	33.371203	1.884000	18.266501
C	37.423303	9.944401	18.070201
C	36.322103	9.296101	18.636701
C	32.981903	4.310500	17.884001
C	30.185802	7.456401	15.513701
C	35.782403	8.299001	16.462701
C	36.913003	8.967001	15.922201
C	37.747003	9.802401	16.687301
C	27.928402	8.416801	15.728001
C	29.042602	7.792001	16.293701
C	35.006103	7.407801	15.545001
H	38.612603	10.315201	16.242001
H	38.612003	10.314701	9.222401
H	33.601403	5.288800	20.060302
H	32.413202	3.096700	2.517700
H	34.215303	2.370900	22.039902
Mg	32.561703	5.495100	15.215501
C	33.679003	0.743400	4.989000
H	33.690503	-0.229000	4.542700
C	33.679603	0.743100	12.008501
H	33.691103	-0.229300	11.562201
C	33.680103	0.742800	19.028001
H	33.691603	-0.229600	18.581701
C	27.890302	8.765101	14.345401
H	27.037702	9.234001	13.900301
C	27.889702	8.765401	7.325901
H	27.037002	9.234101	6.880801

==========

C_I(C-axis)

==========

148

ENERGY = -5576.109253973

C	26.401294	2.233644	8.511403
O	25.588687	2.003690	9.535690
O	26.385359	1.617942	7.466980
C	27.990275	2.555909	11.872706
O	26.877670	1.987926	11.783005
O	28.359124	3.575676	11.093020
N	30.784563	4.249805	7.371702
C	29.636442	4.204950	8.301605
H	30.011160	3.905442	9.288521
C	28.508180	3.275543	7.837888
H	28.851775	2.229989	7.839974
H	28.194520	3.513008	6.808629
N	27.327180	3.357209	8.735082
H	26.047315	2.160459	10.444431
C	26.597670	4.647856	8.591589
H	26.279032	4.796005	7.545475
H	25.718510	4.631410	9.247840
H	27.250667	5.478486	8.890997
H	29.265202	5.232966	8.393693
H	31.214630	3.318312	7.350852
C	30.371481	4.615022	5.997695
H	31.227113	5.019083	5.453568
H	29.927675	3.772199	5.441818
H	29.628197	5.421731	6.060912
N	30.839280	4.174132	14.611379
C	29.667146	4.201029	15.505567
H	30.024707	4.206618	16.543470
H	29.101768	5.124360	15.325912
H	28.991311	3.342239	15.351150
C	30.500764	4.152311	13.176780

H	31.312252	4.651012	12.636258
C	30.304942	2.747074	12.597258
H	31.012710	2.048571	13.072740
H	30.551411	2.766970	11.526677
N	28.954171	2.195169	12.762337
H	27.851656	3.478559	10.167924
C	28.752347	1.066274	13.658392
H	27.690325	0.795233	13.654556
H	29.346782	0.197436	13.328171
H	29.059083	1.331857	14.682587
H	31.369430	3.322083	14.828751
H	29.597384	4.755432	13.011886
Mg	34.197003	6.437400	5.842800
O	31.310702	8.053301	4.968900
O	33.750003	4.620000	6.770501
O	32.357202	6.930901	6.633101
O	32.580103	4.066100	2.644600
O	33.076103	5.541300	4.284200
H	29.072902	8.746601	5.503900
H	34.237903	0.099700	7.002901
H	33.102303	1.789000	3.173900
C	33.682703	3.392000	6.164300
C	29.028302	8.466801	6.557501
C	33.972003	0.951900	6.370000
C	33.962203	2.229200	6.938301
C	31.331202	7.604501	6.177200
C	33.360003	3.196800	4.768300
C	33.370103	1.884600	4.227500
C	32.980703	4.311100	3.845000
Mg	32.561103	5.495400	8.196001
Mg	34.197603	6.437100	12.862301
Mg	32.569403	7.387801	10.519601
O	31.217502	6.788601	9.097901
O	33.912903	6.852001	8.987001
O	31.311302	8.053001	11.988401
O	33.750503	4.619700	13.790001
O	32.357802	6.930501	13.652601
O	32.580603	4.065800	9.664101
O	34.358003	7.918101	11.447401
O	33.076603	5.541000	11.303701
O	35.399503	7.199101	7.316701
H	29.073402	8.746301	12.523401
H	34.181503	2.365100	8.001001
H	34.238403	0.099400	14.022401
H	33.102903	1.788600	10.193401
H	38.031803	10.595001	11.686301
H	36.093003	9.414401	12.680101
H	37.131403	8.785501	7.849201
H	27.059102	8.618701	9.342801
H	29.057302	7.535301	10.336901
C	33.683303	3.391600	13.183801
C	30.174402	7.829701	7.097601
C	29.028802	8.466401	13.577001
C	33.972603	0.951600	13.389501
C	33.962803	2.228800	13.957801
C	31.331802	7.604201	13.196701
C	35.453503	8.475701	10.840901
C	33.360603	3.196500	11.787801
C	33.370603	1.884300	11.247001
C	37.422803	9.944701	11.050701
C	36.321503	9.296401	11.617201
C	32.981303	4.310800	10.864501
C	30.185302	7.456801	8.494201
C	35.781803	8.299301	9.443201
C	36.912403	8.967301	8.902701
C	37.746503	9.802701	9.667901
C	27.927802	8.417201	8.708501
C	29.042102	7.792401	9.274201
C	35.005503	7.408101	8.525501
Mg	32.570003	7.387501	17.539101
O	31.218102	6.788201	16.117401
O	33.862403	6.902701	16.002901
O	33.751103	4.619300	20.809502
O	32.581203	4.065400	16.683601
O	34.358603	7.917801	18.466901
O	33.077203	5.540600	18.323201
O	35.400003	7.198801	14.336201
H	34.182003	2.364800	15.020401
H	34.239003	0.099100	21.041902
H	33.103403	1.788300	17.212901
H	38.032403	10.594701	18.705701
H	36.093503	9.414101	19.699602
H	37.132003	8.785201	14.868701
H	27.059702	8.618401	16.362301

H	29.057902	7.535001	17.356401
C	33.683803	3.391300	20.203302
C	30.175002	7.829401	14.117101
C	33.973103	0.951300	20.409002
C	33.963303	2.228500	20.977302
C	35.454103	8.475401	17.860401
C	33.361103	3.196200	18.807301
C	33.371203	1.884000	18.266501
C	37.423303	9.944401	18.070201
C	36.322103	9.296101	18.636701
C	32.981903	4.310500	17.884001
C	30.185802	7.456401	15.513701
C	35.782403	8.299001	16.462701
C	36.913003	8.967001	15.922201
C	37.747003	9.802401	16.687301
C	27.928402	8.416801	15.728001
C	29.042602	7.792001	16.293701
C	35.006103	7.407801	15.545001
H	38.612603	10.315201	16.242001
H	38.612003	10.314701	9.222401
H	33.601403	5.288800	20.060302
H	32.413202	3.096700	2.517700
H	34.215303	2.370900	22.039902
Mg	32.561703	5.495100	15.215501
C	33.679003	0.743400	4.989000
H	33.690503	-0.229000	4.542700
C	33.679603	0.743100	12.008501
H	33.691103	-0.229300	11.562201
C	33.680103	0.742800	19.028001
H	33.691603	-0.229600	18.581701
C	27.890302	8.765101	14.345401
H	27.037702	9.234001	13.900301
C	27.889702	8.765401	7.325901
H	27.037002	9.234101	6.880801

==========

C_{II}(C-axis)

==========

148

FINAL HEAT OF FORMATION = -5576.119930

C	26.572358	3.287445	9.386205
O	26.958367	2.041655	9.780062
O	25.689410	3.930644	9.969006
C	27.563644	2.838033	12.515925
O	26.593122	2.071618	12.573218
O	27.469790	4.127160	12.092446
N	30.835498	4.184802	7.353680
C	29.724774	4.035163	8.319722
H	30.155062	3.628415	9.243445
C	28.524765	3.171664	7.846956
H	28.605296	2.143073	8.215859
H	28.494872	3.133661	6.747306
N	27.251464	3.735426	8.294109
H	26.517396	1.870424	10.652345
C	26.860356	5.010286	7.697096
H	26.972533	4.932709	6.604467
H	25.813890	5.214816	7.947886
H	27.474717	5.852190	8.055719
H	29.370924	5.048751	8.550016
H	31.310079	3.280952	7.258540
C	30.374487	4.629430	6.021214
H	31.205928	5.080908	5.475682
H	29.934335	3.816711	5.417696
H	29.617705	5.413360	6.157729
N	30.844092	4.217005	14.513427
C	29.748956	4.089869	15.498814
H	30.192799	3.912825	16.486123
H	29.193480	5.036723	15.527183
H	29.046138	3.278571	15.251026
C	30.373273	4.499276	13.143487
H	31.180280	5.006625	12.599904
C	29.980543	3.275686	12.326975
H	30.838229	2.586838	12.272706
H	29.760882	3.607710	11.300569
N	28.844281	2.499711	12.833702
H	26.597043	4.212184	11.625837
C	29.120662	1.179487	13.381804
H	28.176609	0.714196	13.687331
H	29.613237	0.537525	12.631277
H	29.785318	1.270964	14.255921
H	31.367797	3.333529	14.505709
H	29.528685	5.199714	13.207519
Mg	34.197003	6.437400	5.842800

O	31.310702	8.053301	4.968900
O	33.750003	4.620000	6.770501
O	32.357202	6.930901	6.633101
O	32.580103	4.066100	2.644600
O	33.076103	5.541300	4.284200
H	29.072902	8.746601	5.503900
H	34.237903	0.099700	7.002901
H	33.102303	1.789000	3.173900
C	33.682703	3.392000	6.164300
C	29.028302	8.466801	6.557501
C	33.972003	0.951900	6.370000
C	33.962203	2.229200	6.938301
C	31.331202	7.604501	6.177200
C	33.360003	3.196800	4.768300
C	33.370103	1.884600	4.227500
C	32.980703	4.311100	3.845000
Mg	32.561103	5.495400	8.196001
Mg	34.197603	6.437100	12.862301
Mg	32.569403	7.387801	10.519601
O	31.217502	6.788601	9.097901
O	33.912903	6.852001	8.987001
O	31.311302	8.053001	11.988401
O	33.750503	4.619700	13.790001
O	32.357802	6.930501	13.652601
O	32.580603	4.065800	9.664101
O	34.358003	7.918101	11.447401
O	33.076603	5.541000	11.303701
O	35.399503	7.199101	7.316701
H	29.073402	8.746301	12.523401
H	34.181503	2.365100	8.001001
H	34.238403	0.099400	14.022401
H	33.102903	1.788600	10.193401
H	38.031803	10.595001	11.686301
H	36.093003	9.414401	12.680101
H	37.131403	8.785501	7.849201
H	27.059102	8.618701	9.342801
H	29.057302	7.535301	10.336901
C	33.683303	3.391600	13.183801
C	30.174402	7.829701	7.097601
C	29.028802	8.466401	13.577001
C	33.972603	0.951600	13.389501
C	33.962803	2.228800	13.957801
C	31.331802	7.604201	13.196701
C	35.453503	8.475701	10.840901
C	33.360603	3.196500	11.787801
C	33.370603	1.884300	11.247001
C	37.422803	9.944701	11.050701
C	36.321503	9.296401	11.617201
C	32.981303	4.310800	10.864501
C	30.185302	7.456801	8.494201
C	35.781803	8.299301	9.443201
C	36.912403	8.967301	8.902701
C	37.746503	9.802701	9.667901
C	27.927802	8.417201	8.708501
C	29.042102	7.792401	9.274201
C	35.005503	7.408101	8.525501
Mg	32.570003	7.387501	17.539101
O	31.218102	6.788201	16.117401
O	33.862403	6.902701	16.002901
O	33.751103	4.619300	20.809502
O	32.581203	4.065400	16.683601
O	34.358603	7.917801	18.466901
O	33.077203	5.540600	18.323201
O	35.400003	7.198801	14.336201
H	34.182003	2.364800	15.020401
H	34.239003	0.099100	21.041902
H	33.103403	1.788300	17.212901
H	38.032403	10.594701	18.705701
H	36.093503	9.414101	19.699602
H	37.132003	8.785201	14.868701
H	27.059702	8.618401	16.362301
H	29.057902	7.535001	17.356401
C	33.683803	3.391300	20.203302
C	30.175002	7.829401	14.117101
C	33.973103	0.951300	20.409002
C	33.963303	2.228500	20.977302
C	35.454103	8.475401	17.860401
C	33.361103	3.196200	18.807301
C	33.371203	1.884000	18.266501
C	37.423303	9.944401	18.070201
C	36.322103	9.296101	18.636701
C	32.981903	4.310500	17.884001
C	30.185802	7.456401	15.513701
C	35.782403	8.299001	16.462701

C	36.913003	8.967001	15.922201
C	37.747003	9.802401	16.687301
C	27.928402	8.416801	15.728001
C	29.042602	7.792001	16.293701
C	35.006103	7.407801	15.545001
H	38.612603	10.315201	16.242001
H	38.612003	10.314701	9.222401
H	33.601403	5.288800	20.060302
H	32.413202	3.096700	2.517700
H	34.215303	2.370900	22.039902
Mg	32.561703	5.495100	15.215501
C	33.679003	0.743400	4.989000
H	33.690503	-0.229000	4.542700
C	33.679603	0.743100	12.008501
H	33.691103	-0.229300	11.562201
C	33.680103	0.742800	19.028001
H	33.691603	-0.229600	18.581701
C	27.890302	8.765101	14.345401
H	27.037702	9.234001	13.900301
C	27.889702	8.765401	7.325901
H	27.037002	9.234101	6.880801

==========

A_0 (AB-Fragment)

==========

242

ENERGY = -9856.959041563

Mg	34.211003	6.449400	5.852500
O	31.324702	8.065301	4.978600
O	33.764003	4.632000	6.780201
O	32.371202	6.942901	6.642801
O	32.594103	4.078100	2.654300
O	33.090103	5.553300	4.293900
H	29.086902	8.758601	5.513600
H	34.251903	0.111700	7.012601
H	33.116303	1.801000	3.183600
C	33.696703	3.404000	6.174000
C	29.042302	8.478801	6.567201
C	33.986003	0.963900	6.379700
C	33.976203	2.241200	6.948001
C	31.345202	7.616501	6.186900
C	33.374003	3.208800	4.778000
C	33.384103	1.896600	4.237200
C	33.693003	0.755400	4.998700
C	32.994703	4.323100	3.854700
Mg	32.575103	5.507400	8.205701
Mg	34.211603	6.449100	12.872001
Mg	32.583403	7.399801	10.529301
O	31.231502	6.800601	9.107601
O	33.926903	6.864001	8.996701
O	31.325302	8.065001	11.998101
O	33.764503	4.631700	13.799701
O	32.371802	6.942501	13.662301
O	32.594603	4.077800	9.673801
O	34.372003	7.930101	11.457101
O	33.090603	5.553000	11.313401
O	35.413503	7.211101	7.326401
H	29.087402	8.758301	12.533101
H	34.195503	2.377100	8.010701
H	34.252403	0.111400	14.032101
H	33.116903	1.800600	10.203101
H	38.045803	10.607001	11.696001
H	36.107003	9.426401	12.689801
H	37.145403	8.797501	7.858901
H	27.073102	8.630701	9.352501
H	29.071302	7.547301	10.346601
C	33.697303	3.403600	13.193501
C	30.188402	7.841701	7.107301
C	29.042802	8.478401	13.586701
C	27.903702	8.777401	7.335601
C	33.986603	0.963600	13.399201
C	33.976803	2.240800	13.967501
C	31.345802	7.616201	13.206401
C	35.467503	8.487701	10.850601
C	33.374603	3.208500	11.797501
C	33.384603	1.896300	11.256701
C	33.693603	0.755100	12.018201
C	37.436803	9.956701	11.060401
C	36.335503	9.308401	11.626901
C	32.995303	4.322800	10.874201
C	30.199302	7.468801	8.503901
C	35.795803	8.311301	9.452901
C	36.926403	8.979301	8.912401
C	37.760503	9.814701	9.677601

C	27.941802	8.429201	8.718201
C	29.056102	7.804401	9.283901
C	35.019503	7.420101	8.535201
Mg	32.575703	5.507100	15.225201
Mg	32.584003	7.399501	17.548801
O	31.232102	6.800201	16.127101
O	33.927503	6.863601	16.016201
O	33.765103	4.631300	20.819202
O	32.595203	4.077400	16.693301
O	34.372603	7.929801	18.476601
O	33.091203	5.552600	18.332901
O	35.414003	7.210801	14.345901
H	34.196003	2.376800	15.030101
H	34.253003	0.111100	21.051602
H	33.117403	1.800300	17.222601
H	38.046403	10.606701	18.715401
H	36.107503	9.426101	19.709302
H	37.146003	8.797201	14.878401
H	27.073702	8.630401	16.372001
H	29.071902	7.547001	17.366101
C	33.697803	3.403300	20.213002
C	30.189002	7.841401	14.126801
C	27.904302	8.777101	14.355101
C	33.987103	0.963300	20.418702
C	33.977303	2.240500	20.987002
C	35.468103	8.487401	17.870101
C	33.375103	3.208200	18.817001
C	33.385203	1.896000	18.276201
C	33.694103	0.754800	19.037701
C	37.437303	9.956401	18.079901
C	36.336103	9.308101	18.646401
C	32.995903	4.322500	17.893701
C	30.199802	7.468401	15.523401
C	35.796403	8.311001	16.472401
C	36.927003	8.979001	15.931901
C	37.761003	9.814401	16.697001
C	27.942402	8.428801	15.737701
C	29.056602	7.804001	16.303401
C	35.020103	7.419801	15.554701
Mg	32.552003	-7.256401	5.858200
O	34.343603	-7.773401	4.956400
O	33.050903	-5.407400	5.067300
O	33.751603	-4.488900	2.606800
O	32.608203	-3.946400	6.737601
H	29.030902	-7.418201	6.053300
H	34.233003	0.031200	2.368000
H	34.179903	-2.238200	1.374100
H	36.070403	-9.270801	3.717400
H	38.007803	-10.459601	4.711500
H	33.116103	-1.653300	6.205100
C	35.766903	-8.156201	6.956601
C	37.719603	-9.667001	6.728301
C	33.686803	-3.261300	3.213400
C	33.974303	-0.821400	3.003600
C	33.963503	-2.099300	2.437100
C	35.438403	-8.333201	5.560000
C	33.369803	-3.065200	4.611000
C	33.383103	-1.752100	5.151600
C	33.689503	-0.612100	4.386400
C	37.398903	-9.808101	5.345700
C	36.300703	-9.155501	4.780100
C	32.986203	-4.183100	5.528800
Mg	32.552503	-7.256701	12.877701
Mg	32.549703	-5.368600	8.211501
Mg	34.187203	-6.303300	10.554201
O	34.344203	-7.773701	11.975901
O	33.051403	-5.407700	12.086801
O	35.392303	-7.060301	9.085401
O	33.752103	-4.489200	9.626301
O	32.334202	-6.787501	9.770101
O	32.608803	-3.946800	13.757101
O	31.199402	-6.664501	7.283801
O	33.897003	-6.715201	7.421101
O	31.304602	-7.954601	11.409601
H	37.111703	-8.651701	8.550401
H	27.040802	-8.502101	7.051401
H	29.031402	-7.418601	13.072801
H	34.233503	0.030900	9.387501
H	29.071502	-8.640901	10.880301
H	34.180503	-2.238500	8.393601
H	36.071003	-9.271101	10.736901
H	38.008403	-10.459901	11.731001
H	33.116703	-1.653600	13.224601
C	30.169502	-7.336801	7.889901

C	35.767403	-8.156501	13.976101
C	36.891603	-8.830201	7.496801
C	37.720103	-9.667301	13.747801
C	27.911702	-8.306201	7.684301
C	29.022802	-7.676101	7.116001
C	34.993403	-7.267001	7.877101
C	33.687303	-3.261600	10.232901
C	30.161902	-7.713801	9.285901
C	29.020402	-8.361201	9.826801
C	27.877602	-8.664201	9.065201
C	33.974903	-0.821700	10.023101
C	33.964003	-2.099600	9.456601
C	31.316502	-7.485101	10.209201
C	35.439003	-8.333501	12.579501
C	33.370403	-3.065500	11.630501
C	33.383603	-1.752400	12.171101
C	33.690103	-0.612400	11.405901
C	37.399403	-9.808401	12.365201
C	36.301303	-9.155801	11.799601
C	32.986803	-4.183400	12.548301
Mg	32.550303	-5.369000	15.231001
Mg	34.187803	-6.303600	17.573701
O	33.052003	-5.408100	19.106301
O	35.392903	-7.060601	16.104901
O	33.752703	-4.489500	16.645801
O	32.334802	-6.787801	16.789601
O	32.609303	-3.947100	20.776602
O	31.199902	-6.664801	14.303301
O	33.897603	-6.715501	14.440601
O	31.305202	-7.954901	18.429101
H	37.112203	-8.652001	15.569801
H	27.041302	-8.502401	14.070901
H	34.234103	0.030600	16.407001
H	29.072002	-8.641201	17.899801
H	34.181103	-2.238800	15.413101
H	33.117303	-1.654000	20.244102
C	30.170102	-7.337101	14.909401
C	36.892203	-8.830501	14.516301
C	27.912302	-8.306601	14.703801
C	29.023302	-7.676401	14.135501
C	34.994003	-7.267301	14.896601
C	33.687903	-3.262000	17.252401
C	30.162402	-7.714101	16.305401
C	29.021002	-8.361501	16.846301
C	27.878202	-8.664601	16.084701
C	33.975403	-0.822000	17.042601
C	33.964603	-2.099900	16.476101
C	31.317102	-7.485401	17.228801
C	33.370903	-3.065900	18.650001
C	33.384203	-1.752700	19.190601
C	33.690603	-0.612700	18.425401
C	32.987303	-4.183700	19.567802
H	38.554703	-10.176301	7.162101
H	38.555203	-10.176601	14.181601
H	38.598403	10.319501	16.262801
H	38.598003	10.319701	9.243501
H	34.185303	2.347500	22.031102
H	27.004002	-9.156701	16.534601
H	27.001102	-9.158201	9.509401
H	27.023702	9.266201	13.912901
H	27.025402	9.264601	6.887701
H	33.617503	5.299300	20.070502
H	33.590703	-5.155400	3.355200
H	31.905102	7.455201	4.402700
H	31.881602	-7.349401	19.011501
N	36.310666	5.556629	12.206146
C	36.933684	4.744953	13.279868
H	36.705460	5.243106	14.232894
C	38.448546	4.549461	13.158732
H	38.939993	5.545291	13.032025
H	38.690446	3.964709	12.255203
N	38.945573	3.804595	14.307576
H	38.722879	4.311129	15.167420
C	40.375299	3.525129	14.251279
H	41.016609	4.425786	14.134443
H	40.683473	2.999462	15.166381
H	40.584140	2.857295	13.400806
H	36.438035	3.764333	13.297848
H	36.813147	6.452423	12.174760
C	36.434855	4.916209	10.879962
H	37.474631	4.848404	10.518068
H	36.024123	3.899471	10.939258
H	35.846952	5.475661	10.144241
N	36.282765	-5.412874	11.240146

C	36.926801	-4.613912	10.169439
H	36.719902	-5.125807	9.219041
C	38.438027	-4.414658	10.322183
H	38.925736	-5.407459	10.484142
H	38.657498	-3.809455	11.217717
N	38.965016	-3.696403	9.169838
H	38.770417	-4.225996	8.317031
C	40.391295	-3.409164	9.262780
H	41.031977	-4.303260	9.425685
H	40.726749	-2.909584	8.342718
H	40.570325	-2.716398	10.099893
H	36.429697	-3.634736	10.127397
H	36.779590	-6.311342	11.285297
C	36.393953	-4.764431	12.563775
H	37.427826	-4.714485	12.945408
H	36.004162	-3.740573	12.489999
H	35.780472	-5.305747	13.292246

==========

$A_{I'}$ (AB-Fragment)

==========

242

ENERGY = -9856.942211623

Mg	34.211006	6.449400	5.852500
O	31.324704	8.065302	4.978600
O	33.764006	4.632000	6.780202
O	32.371204	6.942902	6.642802
O	32.594106	4.078100	2.654300
O	33.090106	5.553300	4.293900
H	29.086904	8.758602	5.513600
H	34.251906	0.111700	7.012602
H	33.116306	1.801000	3.183600
C	33.696706	3.404000	6.174000
C	29.042304	8.478802	6.567202
C	33.986006	0.963900	6.379700
C	33.976206	2.241200	6.948002
C	31.345204	7.616502	6.186900
C	33.374006	3.208800	4.778000
C	33.384106	1.896600	4.237200
C	33.693006	0.755400	4.998700
C	32.994706	4.323100	3.854700
Mg	32.575106	5.507400	8.205702
Mg	34.211606	6.449100	12.872002
Mg	32.583406	7.399802	10.529302
O	31.231504	6.800602	9.107602
O	33.926906	6.864002	8.996702
O	31.325304	8.065002	11.998102
O	33.764506	4.631700	13.799702
O	32.371804	6.942502	13.662302
O	32.594606	4.077800	9.673802
O	34.372006	7.930102	11.457102
O	33.090606	5.553000	11.313402
O	35.413506	7.211102	7.326402
H	29.087404	8.758302	12.533102
H	34.195506	2.377100	8.010702
H	34.252406	0.111400	14.032102
H	33.116906	1.800600	10.203102
H	38.045806	10.607002	11.696002
H	36.107006	9.426402	12.689802
H	37.145406	8.797502	7.858902
H	27.073104	8.630702	9.352502
H	29.071304	7.547302	10.346602
C	33.697306	3.403600	13.193502
C	30.188404	7.841702	7.107302
C	29.042804	8.478402	13.586702
C	27.903704	8.777402	7.335602
C	33.986606	0.963600	13.399202
C	33.976806	2.240800	13.967502
C	31.345804	7.616202	13.206402
C	35.467506	8.487702	10.850602
C	33.374606	3.208500	11.797502
C	33.384606	1.896300	11.256702
C	33.693606	0.755100	12.018202
C	37.436806	9.956702	11.060402
C	36.335506	9.308402	11.626902
C	32.995306	4.322800	10.874202
C	30.199304	7.468802	8.503902
C	35.795806	8.311302	9.452902
C	36.926406	8.979302	8.912402
C	37.760506	9.814702	9.677602
C	27.941804	8.429202	8.718202
C	29.056104	7.804402	9.283902
C	35.019506	7.420102	8.535202
Mg	32.575706	5.507100	15.225202

Mg	32.584006	7.399502	17.548802
O	31.232104	6.800202	16.127102
O	33.927506	6.863602	16.016202
O	33.765106	4.631300	20.819204
O	32.595206	4.077400	16.693302
O	34.372606	7.929802	18.476602
O	33.091206	5.552600	18.332902
O	35.414006	7.210802	14.345902
H	34.196006	2.376800	15.030102
H	34.253006	0.111100	21.051604
H	33.117406	1.800300	17.222602
H	38.046406	10.606702	18.715402
H	36.107506	9.426102	19.709304
H	37.146006	8.797202	14.878402
H	27.073704	8.630402	16.372002
H	29.071904	7.547002	17.366102
C	33.697806	3.403300	20.213004
C	30.189004	7.841402	14.126802
C	27.904304	8.777102	14.355102
C	33.987106	0.963300	20.418704
C	33.977306	2.240500	20.987004
C	35.468106	8.487402	17.870102
C	33.375106	3.208200	18.817002
C	33.385206	1.896000	18.276202
C	33.694106	0.754800	19.037702
C	37.437306	9.956402	18.079902
C	36.336106	9.308102	18.646402
C	32.995906	4.322500	17.893702
C	30.199804	7.468402	15.523402
C	35.796406	8.311002	16.472402
C	36.927006	8.979002	15.931902
C	37.761006	9.814402	16.697002
C	27.942404	8.428802	15.737702
C	29.056604	7.804002	16.303402
C	35.020106	7.419802	15.554702
Mg	32.552006	-7.256402	5.858200
O	34.343606	-7.773402	4.956400
O	33.050906	-5.407400	5.067300
O	33.751606	-4.488900	2.606800
O	32.608206	-3.946400	6.737602
H	29.030904	-7.418202	6.053300
H	34.233006	0.031200	2.368000
H	34.179906	-2.238200	1.374100
H	36.070406	-9.270802	3.717400
H	38.007806	-10.459602	4.711500
H	33.116106	-1.653300	6.205100
C	35.766906	-8.156202	6.956602
C	37.719606	-9.667002	6.728302
C	33.686806	-3.261300	3.213400
C	33.974306	-0.821400	3.003600
C	33.963506	-2.099300	2.437100
C	35.438406	-8.333202	5.560000
C	33.369806	-3.065200	4.611000
C	33.383106	-1.752100	5.151600
C	33.689506	-0.612100	4.386400
C	37.398906	-9.808102	5.345700
C	36.300706	-9.155502	4.780100
C	32.986206	-4.183100	5.528800
Mg	32.552506	-7.256702	12.877702
Mg	32.549706	-5.368600	8.211502
Mg	34.187206	-6.303300	10.554202
O	34.344206	-7.773702	11.975902
O	33.051406	-5.407700	12.086802
O	35.392306	-7.060302	9.085402
O	33.752106	-4.489200	9.626302
O	32.334204	-6.787502	9.770102
O	32.608806	-3.946800	13.757102
O	31.199404	-6.664502	7.283802
O	33.897006	-6.715202	7.421102
O	31.304604	-7.954602	11.409602
H	37.111706	-8.651702	8.550402
H	27.040804	-8.502102	7.051402
H	29.031404	-7.418602	13.072802
H	34.233506	0.030900	9.387502
H	29.071504	-8.640902	10.880302
H	34.180506	-2.238500	8.393602
H	36.071006	-9.271102	10.736902
H	38.008406	-10.459902	11.731002
H	33.116706	-1.653600	13.224602
C	30.169504	-7.336802	7.889902
C	35.767406	-8.156502	13.976102
C	36.891606	-8.830202	7.496802
C	37.720106	-9.667302	13.747802
C	27.911704	-8.306202	7.684302

C	29.022804	-7.676102	7.116002
C	34.993406	-7.267002	7.877102
C	33.687306	-3.261600	10.232902
C	30.161904	-7.713802	9.285902
C	29.020404	-8.361202	9.826802
C	27.877604	-8.664202	9.065202
C	33.974906	-0.821700	10.023102
C	33.964006	-2.099600	9.456602
C	31.316504	-7.485102	10.209202
C	35.439006	-8.333502	12.579502
C	33.370406	-3.065500	11.630502
C	33.383606	-1.752400	12.171102
C	33.690106	-0.612400	11.405902
C	37.399406	-9.808402	12.365202
C	36.301306	-9.155802	11.799602
C	32.986806	-4.183400	12.548302
Mg	32.550306	-5.369000	15.231002
Mg	34.187806	-6.303600	17.573702
O	33.052006	-5.408100	19.106302
O	35.392906	-7.060602	16.104902
O	33.752706	-4.489500	16.645802
O	32.334804	-6.787802	16.789602
O	32.609306	-3.947100	20.776604
O	31.199904	-6.664802	14.303302
O	33.897606	-6.715502	14.440602
O	31.305204	-7.954902	18.429102
H	37.112206	-8.652002	15.569802
H	27.041304	-8.502402	14.070902
H	34.234106	0.030600	16.407002
H	29.072004	-8.641202	17.899802
H	34.181106	-2.238800	15.413102
H	33.117306	-1.654000	20.244104
C	30.170104	-7.337102	14.909402
C	36.892206	-8.830502	14.516302
C	27.912304	-8.306602	14.703802
C	29.023304	-7.676402	14.135502
C	34.994006	-7.267302	14.896602
C	33.687906	-3.262000	17.252402
C	30.162404	-7.714102	16.305402
C	29.021004	-8.361502	16.846302
C	27.878204	-8.664602	16.084702
C	33.975406	-0.822000	17.042602
C	33.964606	-2.099900	16.476102
C	31.317104	-7.485402	17.228802
C	33.370906	-3.065900	18.650002
C	33.384206	-1.752700	19.190602
C	33.690606	-0.612700	18.425402
C	32.987306	-4.183700	19.567804
H	38.554706	-10.176302	7.162102
H	38.555206	-10.176602	14.181602
H	38.598406	10.319502	16.262802
H	38.598006	10.319702	9.243502
H	34.185306	2.347500	22.031104
H	27.004004	-9.156702	16.534602
H	27.001104	-9.158202	9.509402
H	27.023704	9.266202	13.912902
H	27.025404	9.264602	6.887702
H	33.617506	5.299300	20.070504
H	33.590706	-5.155400	3.355200
H	31.905104	7.455202	4.402700
H	31.881604	-7.349402	19.011502
N	36.472655	5.482312	12.393701
C	36.869645	4.199756	13.043805
H	37.896062	4.301519	13.447590
C	36.846643	2.982310	12.100783
H	37.567106	3.136599	11.280721
H	35.852938	2.883207	11.644162
N	37.184222	1.706670	12.735468
H	36.485385	1.497644	13.450759
C	38.534718	1.639689	13.292988
H	38.749312	2.361123	14.107792
H	38.717911	0.625836	13.680438
H	39.261163	1.822367	12.484375
H	36.187450	4.026375	13.888351
H	36.740581	6.209225	13.067845
C	37.267776	5.716840	11.171642
H	38.325542	5.415031	11.304198
H	36.851608	5.145195	10.329903
H	37.243909	6.779624	10.913158
N	36.486457	-5.290104	11.045693
C	36.933831	-3.975591	10.501605
H	38.000001	-4.047323	10.204838
C	36.831976	-2.805589	11.490176
H	37.099643	-3.156585	12.498769

H	35.791113	-2.446265	11.530156
N	37.786393	-1.737501	11.148457
H	37.680746	-0.988924	11.839869
C	37.553437	-1.142163	9.830604
H	36.519209	-0.774766	9.679479
H	38.245588	-0.298222	9.695931
H	37.769223	-1.880693	9.043080
H	36.336560	-3.774702	9.600575
H	36.719155	-5.959284	10.302789
C	37.292854	-5.665336	12.227188
H	38.330404	-5.287540	12.148494
H	36.848145	-5.258043	13.146388
H	37.327073	-6.755473	12.320369

==========

C_{II} (AB-Fragment)

==========

248

ENERGY = -10233.94436184

Mg	34.211003	6.449400	5.852500
O	31.324702	8.065301	4.978600
O	33.764003	4.632000	6.780201
O	32.371202	6.942901	6.642801
O	32.594103	4.078100	2.654300
O	33.090103	5.553300	4.293900
H	29.086902	8.758601	5.513600
H	34.251903	0.111700	7.012601
H	33.116303	1.801000	3.183600
C	33.696703	3.404000	6.174000
C	29.042302	8.478801	6.567201
C	33.986003	0.963900	6.379700
C	33.976203	2.241200	6.948001
C	31.345202	7.616501	6.186900
C	33.374003	3.208800	4.778000
C	33.384103	1.896600	4.237200
C	33.693003	0.755400	4.998700
C	32.994703	4.323100	3.854700
Mg	32.575103	5.507400	8.205701
Mg	34.211603	6.449100	12.872001
Mg	32.583403	7.399801	10.529301
O	31.231502	6.800601	9.107601
O	33.926903	6.864001	8.996701
O	31.325302	8.065001	11.998101
O	33.764503	4.631700	13.799701
O	32.371802	6.942501	13.662301
O	32.594603	4.077800	9.673801
O	34.372003	7.930101	11.457101
O	33.090603	5.553000	11.313401
O	35.413503	7.211101	7.326401
H	29.087402	8.758301	12.533101
H	34.195503	2.377100	8.010701
H	34.252403	0.111400	14.032101
H	33.116903	1.800600	10.203101
H	38.045803	10.607001	11.696001
H	36.107003	9.426401	12.689801
H	37.145403	8.797501	7.858901
H	27.073102	8.630701	9.352501
H	29.071302	7.547301	10.346601
C	33.697303	3.403600	13.193501
C	30.188402	7.841701	7.107301
C	29.042802	8.478401	13.586701
C	27.903702	8.777401	7.335601
C	33.986603	0.963600	13.399201
C	33.976803	2.240800	13.967501
C	31.345802	7.616201	13.206401
C	35.467503	8.487701	10.850601
C	33.374603	3.208500	11.797501
C	33.384603	1.896300	11.256701
C	33.693603	0.755100	12.018201
C	37.436803	9.956701	11.060401
C	36.335503	9.308401	11.626901
C	32.995303	4.322800	10.874201
C	30.199302	7.468801	8.503901
C	35.795803	8.311301	9.452901
C	36.926403	8.979301	8.912401
C	37.760503	9.814701	9.677601
C	27.941802	8.429201	8.718201
C	29.056102	7.804401	9.283901
C	35.019503	7.420101	8.535201
Mg	32.575703	5.507100	15.225201
Mg	32.584003	7.399501	17.548801
O	31.232102	6.800201	16.127101
O	33.927503	6.863601	16.016201
O	33.765103	4.631300	20.819202

O	32.595203	4.077400	16.693301
O	34.372603	7.929801	18.476601
O	33.091203	5.552600	18.332901
O	35.414003	7.210801	14.345901
H	34.196003	2.376800	15.030101
H	34.253003	0.111100	21.051602
H	33.117403	1.800300	17.222601
H	38.046403	10.606701	18.715401
H	36.107503	9.426101	19.709302
H	37.146003	8.797201	14.878401
H	27.073702	8.630401	16.372001
H	29.071902	7.547001	17.366101
C	33.697803	3.403300	20.213002
C	30.189002	7.841401	14.126801
C	27.904302	8.777101	14.355101
C	33.987103	0.963300	20.418702
C	33.977303	2.240500	20.987002
C	35.468103	8.487401	17.870101
C	33.375103	3.208200	18.817001
C	33.385203	1.896000	18.276201
C	33.694103	0.754800	19.037701
C	37.437303	9.956401	18.079901
C	36.336103	9.308101	18.646401
C	32.995903	4.322500	17.893701
C	30.199802	7.468401	15.523401
C	35.796403	8.311001	16.472401
C	36.927003	8.979001	15.931901
C	37.761003	9.814401	16.697001
C	27.942402	8.428801	15.737701
C	29.056602	7.804001	16.303401
C	35.020103	7.419801	15.554701
Mg	32.552003	-7.256401	5.858200
O	34.343603	-7.773401	4.956400
O	33.050903	-5.407400	5.067300
O	33.751603	-4.488900	2.606800
O	32.608203	-3.946400	6.737601
H	29.030902	-7.418201	6.053300
H	34.233003	0.031200	2.368000
H	34.179903	-2.238200	1.374100
H	36.070403	-9.270801	3.717400
H	38.007803	-10.459601	4.711500
H	33.116103	-1.653300	6.205100
C	35.766903	-8.156201	6.956601
C	37.719603	-9.667001	6.728301
C	33.686803	-3.261300	3.213400
C	33.974303	-0.821400	3.003600
C	33.963503	-2.099300	2.437100
C	35.438403	-8.333201	5.560000
C	33.369803	-3.065200	4.611000
C	33.383103	-1.752100	5.151600
C	33.689503	-0.612100	4.386400
C	37.398903	-9.808101	5.345700
C	36.300703	-9.155501	4.780100
C	32.986203	-4.183100	5.528800
Mg	32.552503	-7.256701	12.877701
Mg	32.549703	-5.368600	8.211501
Mg	34.187203	-6.303300	10.554201
O	34.344203	-7.773701	11.975901
O	33.051403	-5.407700	12.086801
O	35.392303	-7.060301	9.085401
O	33.752103	-4.489200	9.626301
O	32.334202	-6.787501	9.770101
O	32.608803	-3.946800	13.757101
O	31.199402	-6.664501	7.283801
O	33.897003	-6.715201	7.421101
O	31.304602	-7.954601	11.409601
H	37.111703	-8.651701	8.550401
H	27.040802	-8.502101	7.051401
H	29.031402	-7.418601	13.072801
H	34.233503	0.030900	9.387501
H	29.071502	-8.640901	10.880301
H	34.180503	-2.238500	8.393601
H	36.071003	-9.271101	10.736901
H	38.008403	-10.459901	11.731001
H	33.116703	-1.653600	13.224601
C	30.169502	-7.336801	7.889901
C	35.767403	-8.156501	13.976101
C	36.891603	-8.830201	7.496801
C	37.720103	-9.667301	13.747801
C	27.911702	-8.306201	7.684301
C	29.022802	-7.676101	7.116001
C	34.993403	-7.267001	7.877101
C	33.687303	-3.261600	10.232901
C	30.161902	-7.713801	9.285901

C	29.020402	-8.361201	9.826801
C	27.877602	-8.664201	9.065201
C	33.974903	-0.821700	10.023101
C	33.964003	-2.099600	9.456601
C	31.316502	-7.485101	10.209201
C	35.439003	-8.333501	12.579501
C	33.370403	-3.065500	11.630501
C	33.383603	-1.752400	12.171101
C	33.690103	-0.612400	11.405901
C	37.399403	-9.808401	12.365201
C	36.301303	-9.155801	11.799601
C	32.986803	-4.183400	12.548301
Mg	32.550303	-5.369000	15.231001
Mg	34.187803	-6.303600	17.573701
O	33.052003	-5.408100	19.106301
O	35.392903	-7.060601	16.104901
O	33.752703	-4.489500	16.645801
O	32.334802	-6.787801	16.789601
O	32.609303	-3.947100	20.776602
O	31.199902	-6.664801	14.303301
O	33.897603	-6.715501	14.440601
O	31.305202	-7.954901	18.429101
H	37.112203	-8.652001	15.569801
H	27.041302	-8.502401	14.070901
H	34.234103	0.030600	16.407001
H	29.072002	-8.641201	17.899801
H	34.181103	-2.238800	15.413101
H	33.117303	-1.654000	20.244102
C	30.170102	-7.337101	14.909401
C	36.892203	-8.830501	14.516301
C	27.912302	-8.306601	14.703801
C	29.023302	-7.676401	14.135501
C	34.994003	-7.267301	14.896601
C	33.687903	-3.262000	17.252401
C	30.162402	-7.714101	16.305401
C	29.021002	-8.361501	16.846301
C	27.878202	-8.664601	16.084701
C	33.975403	-0.822000	17.042601
C	33.964603	-2.099900	16.476101
C	31.317102	-7.485401	17.228801
C	33.370903	-3.065900	18.650001
C	33.384203	-1.752700	19.190601
C	33.690603	-0.612700	18.425401
C	32.987303	-4.183700	19.567802
H	38.554703	-10.176301	7.162101
H	38.555203	-10.176601	14.181601
H	38.598403	10.319501	16.262801
H	38.598003	10.319701	9.243501
H	34.185303	2.347500	22.031102
H	27.004002	-9.156701	16.534601
H	27.001102	-9.158201	9.509401
H	27.023702	9.266201	13.912901
H	27.025402	9.264601	6.887701
H	33.617503	5.299300	20.070502
H	33.590703	-5.155400	3.355200
H	31.905102	7.455201	4.402700
H	31.881602	-7.349401	19.011501
N	36.306212	5.428098	12.105141
C	36.920295	4.475018	13.060127
H	36.822964	4.919222	14.062392
C	38.400146	4.084875	12.870527
H	38.702244	3.523669	13.769344
H	39.029577	4.986111	12.816211
N	38.705548	3.274088	11.681039
C	39.557717	3.853981	10.646809
H	40.600692	3.940725	10.998178
H	39.537580	3.221973	9.754389
H	39.202000	4.858481	10.376850
H	36.314157	3.559239	13.058000
H	36.862271	6.290984	12.112414
C	36.233818	4.915205	10.719826
H	37.194481	4.926321	10.185233
H	35.872231	3.879673	10.744000
H	35.512929	5.508252	10.150091
N	36.284968	-5.286187	11.338091
C	36.908405	-4.332674	10.390052
H	36.816961	-4.774136	9.386047
C	38.387976	-3.947247	10.592056
H	38.699452	-3.385215	9.697045
H	39.014467	-4.850296	10.649860
N	38.684492	-3.139535	11.786023
C	39.524490	-3.722577	12.828584
H	40.576917	-3.783843	12.500740
H	39.472529	-3.108362	13.732222

H	39.180532	-4.738039	13.070223
H	36.304777	-3.415172	10.390107
H	36.836126	-6.152149	11.328948
C	36.209209	-4.779569	12.725547
H	37.165016	-4.808766	13.268200
H	35.864230	-3.738384	12.704912
H	35.474420	-5.363936	13.286405
C	38.425179	-1.797769	11.756365
C	38.437627	1.933872	11.709000
O	37.973050	1.367460	12.722898
O	37.973168	-1.227645	10.738873
O	38.710475	1.292724	10.565316
H	38.376246	0.325837	10.633066
O	38.692751	-1.159133	12.902839
H	38.365339	-0.190247	12.832994

==========

CO_2 (No Fragment)

==========

3

ENERGY = -188.4692651719

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.172169
O	0.000000	0.000000	-1.172169

==========

mmen (No Fragment)

==========

18

ENERGY = -268.8699345872

N	0.818484	-5.403309	2.852458
H	-0.059038	-5.130045	3.300229
C	1.924865	-4.628281	3.409902
H	2.838622	-4.853692	2.836265
H	1.712794	-3.555242	3.291920
H	2.145825	-4.820137	4.481431
C	0.995946	-6.848335	2.962512
H	1.960561	-7.114366	2.499275
H	0.207550	-7.340310	2.364550
C	0.958742	-7.416546	4.388048
H	-0.007524	-7.119339	4.865048
H	1.761398	-6.962061	4.993511
N	1.165014	-8.858973	4.380707
H	0.479341	-9.290861	3.756270
C	1.051553	-9.448425	5.710633
H	0.095628	-9.209840	6.229467
H	1.148980	-10.542121	5.643266
H	1.873262	-9.076028	6.343714

8. References

1. McDonald, T. M.; Lee, W. R.; Mason, J. A.; Wiers, B. M.; Hong, C. S.; Long, J. R. *J. Am. Chem. Soc.* **2012**, *134*, 7056.
2. Caplow, M. *J. Am. Chem. Soc.* **1968**, *90*, 6795.
3. Danckwerts, P. V. *Chem. Eng. Sci.* **1979**, *34*, 443.
4. Vaidya, P. D.; Kenig, E. Y. *Chem. Eng. Technol.* **2007**, *30*, 1467.
5. da Silva, E. F.; Svendsen, H. F. *Ind. Eng. Chem. Res.* **2004**, *43*, 3413.
6. Crooks, J. E.; Donnellan, J. P. *J. Am. Chem. Soc. Perkin Trans. 2* **1989**, 331.
7. Vaidya, P. D.; Kenig, E. Y. *Chem. Eng. Technol.* **2010**, *33*, 1577.
8. Ramachandran, N.; Aboudheir, A.; Idem, R.; Tontiwachwuthikul, P. *Ind. Eng. Chem. Res.* **2006**, *45*, 2608.
9. Hartono, A.; da Silva, E. F.; Svendsen, H. F. *Chem. Eng. Sci.* **2009**, *64*, 3205.
10. Aboudheir, A.; Tontiwachwuthikul, P.; Chakma, A.; Idem, R. *Chem. Eng. Sci.* **2003**, *58*, 5195.
11. Hampe, E. M.; Rudkevich, D. M. *Chem. Commun.* **2002**, 1450.
12. Hampe, E. M.; Rudkevich, D. M. *Tetrahedron* **2003**, *59*, 9619.
13. Soler, J. M.; Artacho, E.; Gale, J. D.; Garcia, A.; Junquera, J.; Ordejon, P.; Sanchez-Portal, D. *J. Phys. -Condens. Mat.* **2002**, *14*, 2745.
14. Roman-Perez, G.; Soler, J. M. *Phys. Rev. Lett.* **2009**, *103*, Artn 096102.
15. Perdew, J. P.; Wang, Y. *Phys. Rev. B* **1992**, *45*, 13244.
16. Perdew, J. P.; Emzerhof, M.; Burke, K. *J. Chem. Phys.* **1996**, *105*, 9982.
17. Perdew, J. P.; Burke, K.; Ernzerhof, M. *Phys. Rev. Lett.* **1996**, *77*, 3865.
18. Grimme, S. *J. Comput. Chem.* **2004**, *25*, 1463.
19. Grimme, S. *J. Comput. Chem.* **2006**, *27*, 1787.
20. Valenzano, L.; Civalleri, B.; Sillar, K.; Sauer, J. *J. Phys. Chem. C.* **2011**, *115*, 21777.
21. Poloni, R.; Smit, B.; Neaton, J. B. *J. Phys. Chem. A.* **2012**, *116*, 4957.
22. Troullier, N.; Martins, J. L. *Phys. Rev. B.* **1991**, *43*, 1993.
23. Junquera, J.; Paz, O.; Sanchez-Portal, D.; Artacho, E. *Phys. Rev. B.* **2001**, *64*, 235111.
24. Moreno, J.; Soler, J. M. *Phys. Rev. B.* **1992**, *45*, 13891.
25. Schafer, A.; Horn, H.; Ahlrichs, R. *J. Chem. Phys.* **1992**, *97*, 2571.
26. Schafer, A.; Huber, C.; Ahlrichs, R. *J. Chem. Phys.* **1994**, *100*, 5829.
27. Ahlrichs, R.; Bar, M.; Haser, M.; Horn, H.; Kolmel, C. *Chem. Phys. Lett.* **1989**, *162*, 165.
28. Perdew, J. P.; Burke, K.; Ernzerhof, M. *Phys. Rev. Lett.* **1997**, *78*, 1396.
29. Ernzerhof, M.; Perdew, J. P. *J. Chem. Phys.* **1998**, *109*, 3313.
30. Adamo, C.; Barone, V. *J. Chem. Phys.* **1999**, *110*, 6158.
31. Zhao, Y.; Truhlar, D. G. *J. Chem. Phys.* **2006**, *125*, 194101.
32. Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215.
33. Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B.* **1988**, *37*, 785.
34. Miehlich, B.; Savin, A.; Stoll, H.; Preuss, H. *Chem. Phys. Lett.* **1989**, *157*, 200.
35. Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648.
36. Vosko, S. H.; Wilk, L.; Nusair, M. *Can. J. Phys.* **1980**, *58*, 1200.
37. Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623.
38. Vydrov, O. A.; Scuseria, G. E. *J. Chem. Phys.* **2006**, *125*, 234109.
39. Vydrov, O. A.; Heyd, J.; Krukau, A.; Scuseria, G. E. *J. Chem. Phys.* **2006**, *125*, 074106.
40. Vydrov, O. A.; Scuseria, G. E.; Perdew, J. P. *J. Chem. Phys.* **2007**, *126*, 154109.
41. Yanai, T.; Tew, D.; Handy, N. *Chem. Phys. Lett.* **2004**, *393*, 51.
42. Lendvay, G.; Mayer, I. Some difficulties in computing BSSE-corrected potential surfaces of chemical reactions. *Chem. Phys. Lett.* **1998**, *297*, 365.