

Conformer interconversion in a switchable porous organic cage

Kim E. Jelfs,^{a*} Florian Schiffmann,^b James T. A. Jones,^a Ben Slater,^b Furio Cora^b and Andrew I. Cooper^{a*}

Supporting Information

Simulation details

Molecular Dynamics for solvent configurations: The solvent molecules were concentrated around the bond subject to rotation and molecular dynamics (MD) calculations at the PM6 level with an NVE ensemble and a timestep of 0.5 fs for a total of 0.5 ps at 300 K followed by a further 0.5 ps at 150 K and then a geometry optimisation. These MD calculations were repeated several times using different starting conformations to sample different solvent arrangements to find the three lowest energy conformations which were then used for the full DFT calculations.

A note on the calculation of frequencies for these systems Due to the size of the system and the solvent molecules it was not possible to perform frequency calculations to confirm the true transition state nature of structures. The flexible nature of the cage molecule also meant that small displacements on the opposite side of the cage could affect the frequencies.

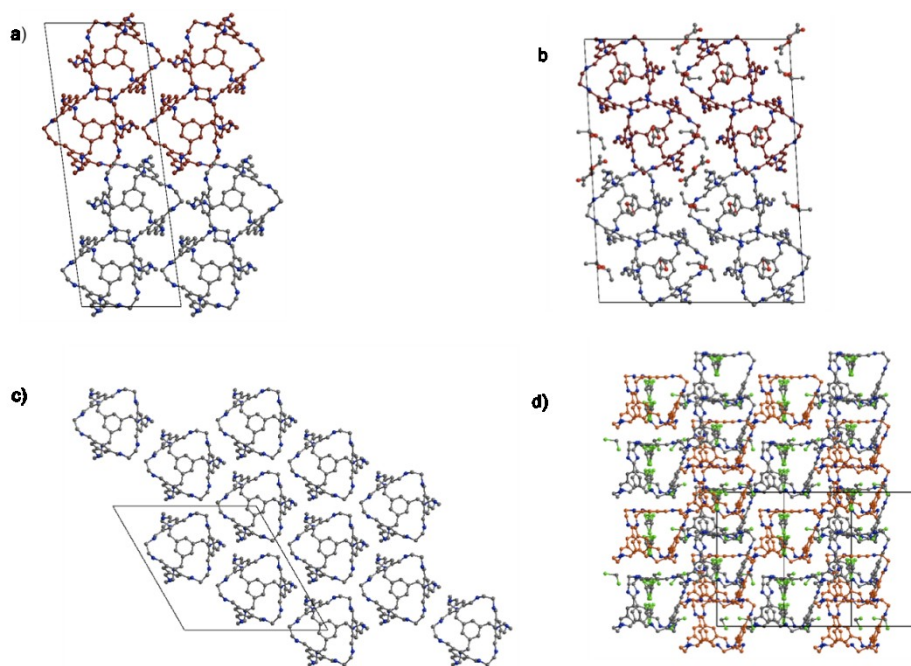


Figure S1 A comparison of the **CC1 α** and **CC1 β** polymorphs; (a) **CC1 α** desolvate structure, a racemate of both tetrahedral cage conformers; (b) **CC1 α .EtOAc** ethyl acetate solvate structure, a racemate (c) **CC1 β** desolvate structure, containing only **1^T-S** conformer (d) **CC1 β .DCM** dichloromethane solvate structure (DCM inside the cage is disordered), with **1^T-S** and **1^{C3}** conformers. Cage **1^T-R** shown in dark red, cage **1^T-S** shown in grey, cage **1^{C3}** shown in orange. Otherwise nitrogen (blue), chlorine (green) and oxygen (red). Hydrogen atoms are omitted for clarity.

Solvent	"H inside" TS	"H outside" TS
Dichloromethane	-28	-61
Methanol	-32	-61
Ethyl acetate	-85	-80
Carbon tetrachloride	-76	-73

Table S1 Binding energies for a single solvent within the TS structures in kJ mol^{-1} . Calculated as $E_b = E(\text{TS}) - S.P.(\text{Cage}) - S.P.(\text{Solvent})$, where $S.P.(\text{Cage})$ and $S.P.(\text{Solvent})$ are the single point energies of the cage and the solvent structure from the TS structure.

Plots of the energy profile for imine bond rotation

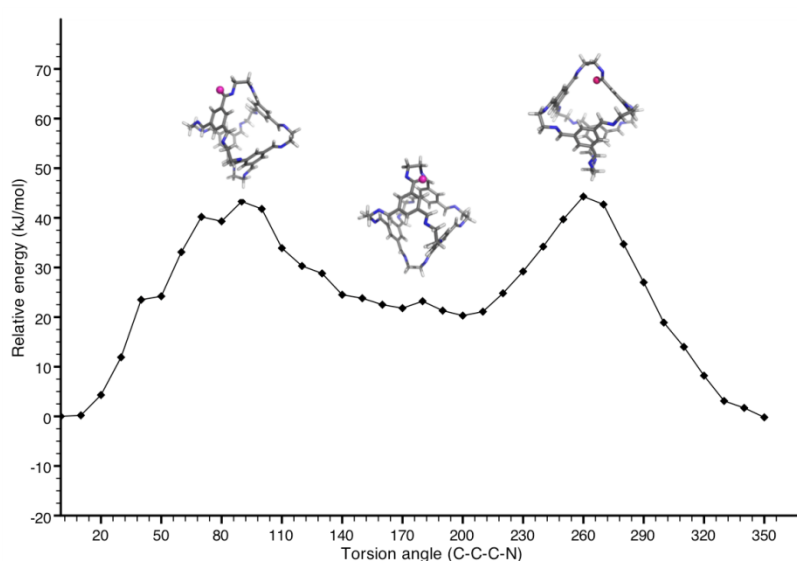


Figure S2 Profile for the rotation about the first bond from the T_d conformer in the gas phase. A torsion angle of 0° is the T_d conformer, at 90° is the transition state where the H was rotated outside of the cage, 180° is the point where the imine bond has flipped, 270° is the transition state where the H was rotated inside of the cage and 360° is back to the T_d conformer. The structures of the transition states and the midpoint are shown with the hydrogen being flipped shown in pink.

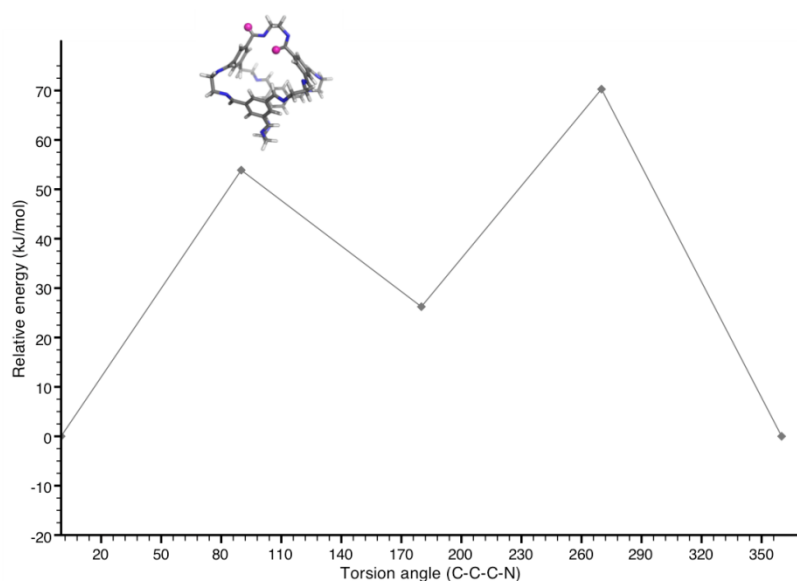


Figure S3 Profile for the simultaneous rotation about the first and second bond from the T_d conformer in the gas phase.

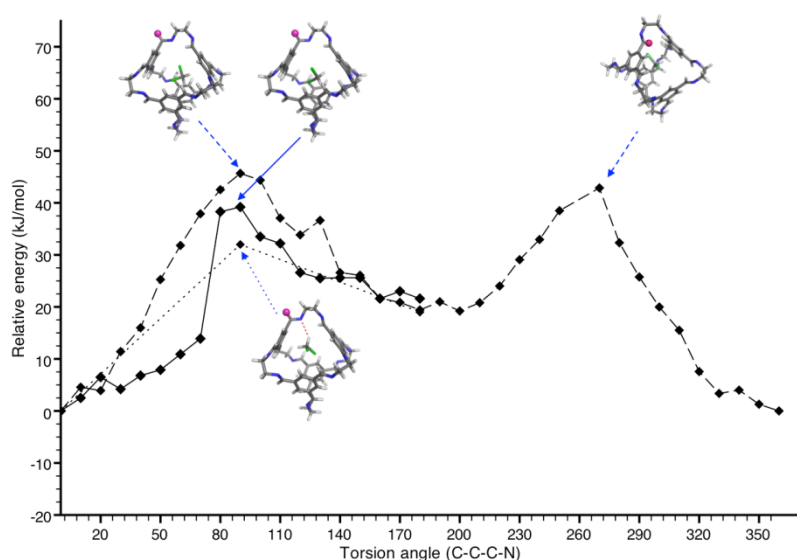


Figure S4 Profile for the rotation about the first bond from the T_d conformer with one dichloromethane (DCM) molecule in the centre of the cage. Several alternative DCM orientations relative to the cage molecule are shown.

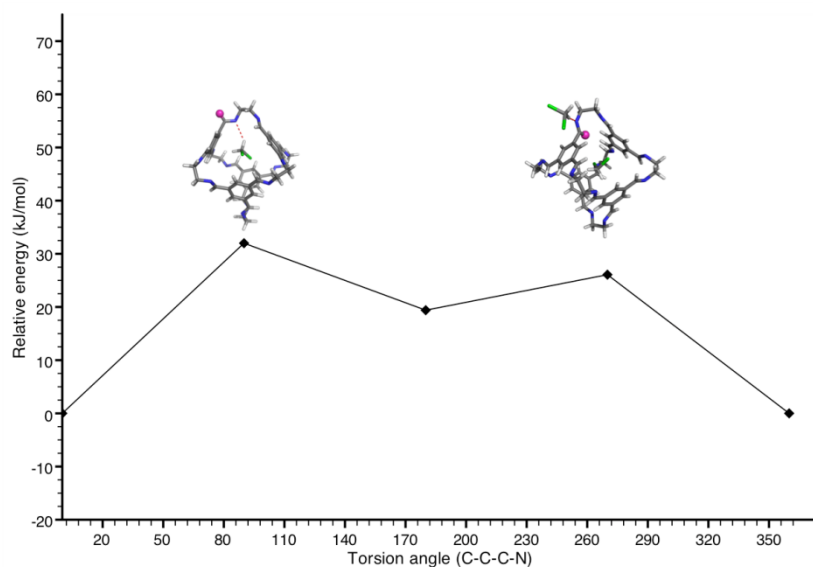


Figure S5 Profile for the rotation about the first bond from the T_d conformer with a microsolvation of 13 DCM molecules. Only key DCM molecules are shown for clarity.

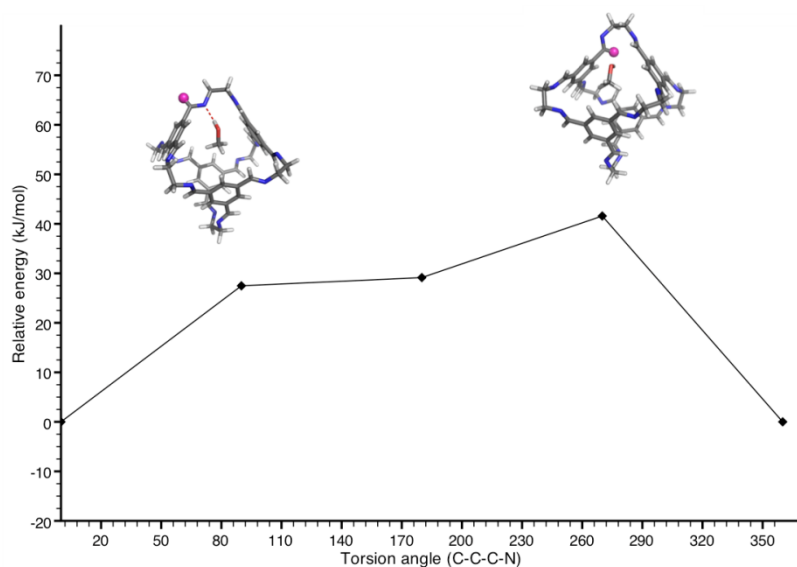


Figure S6 Profile for the rotation about the first bond from the T_d conformer with one methanol molecule in the centre of the cage.

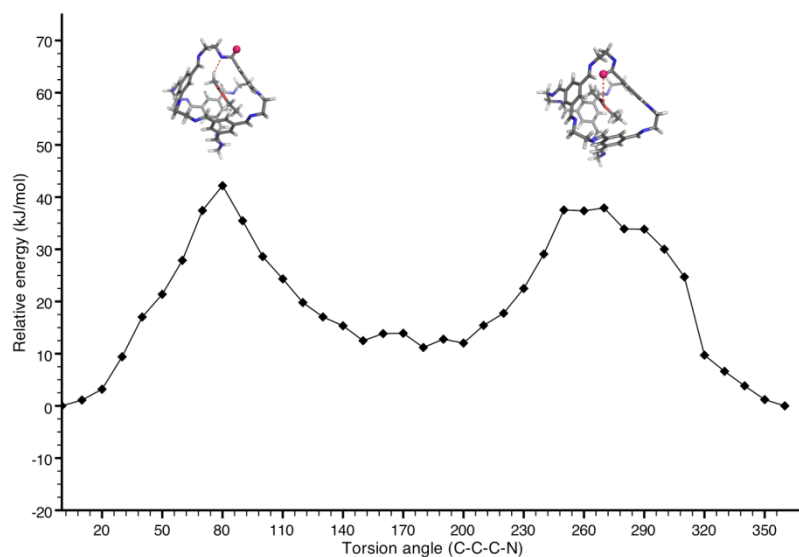


Figure S7 Profile for the rotation about the first bond from the T_d conformer with one ethyl acetate molecule in the centre of the cage.

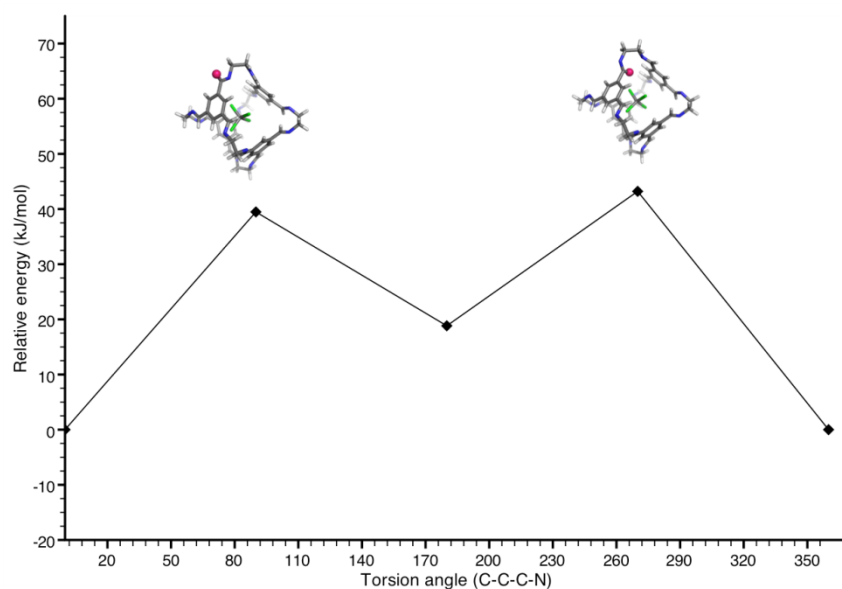


Figure S8 Profile for the rotation about the first bond from the T_d conformer with one carbon tetrachloride molecule in the centre of the cage.

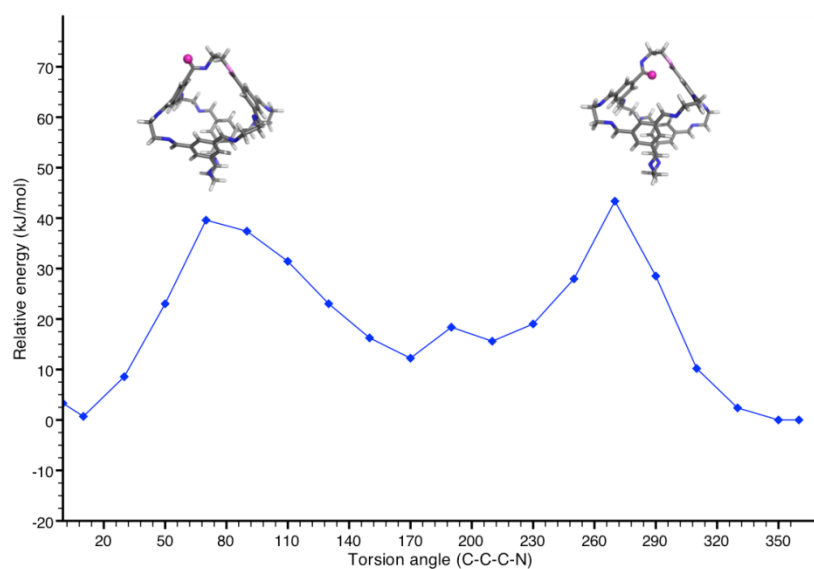


Figure S9 Profile for the rotation about the second bond from the T_d conformer in the gas phase. The nitrogen atom of the imine bond already rotated is shown in purple.

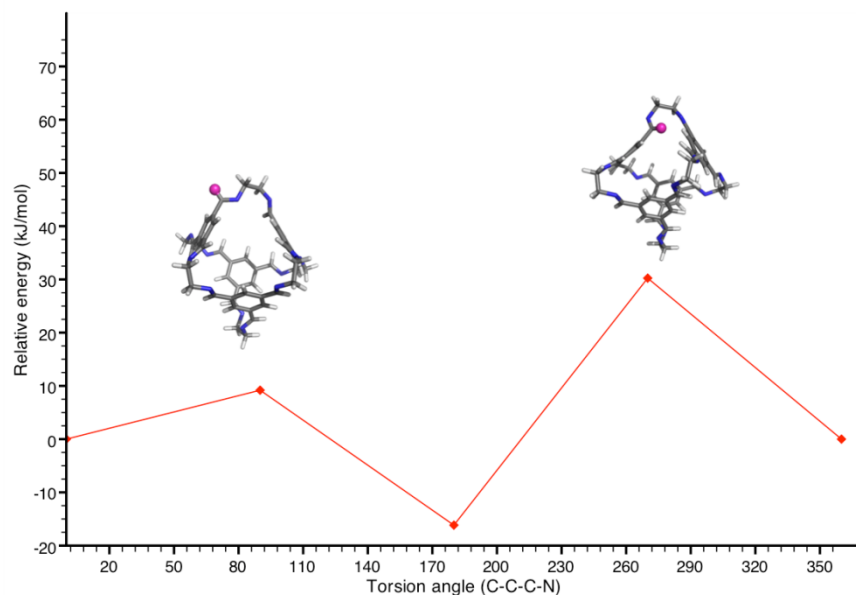
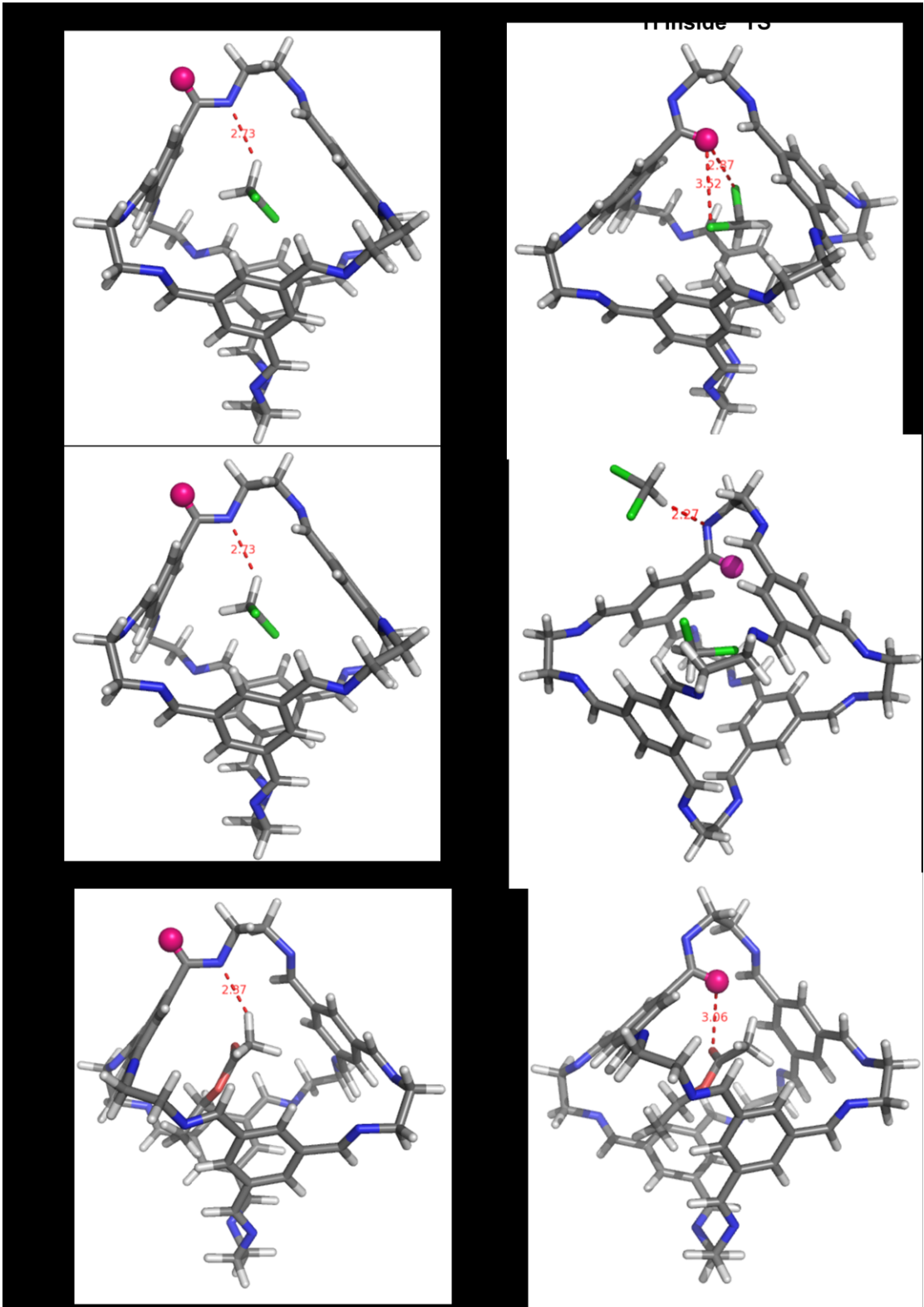


Figure S10 Profile for the rotation about the last bond to form the C_3 conformer in the gas phase.



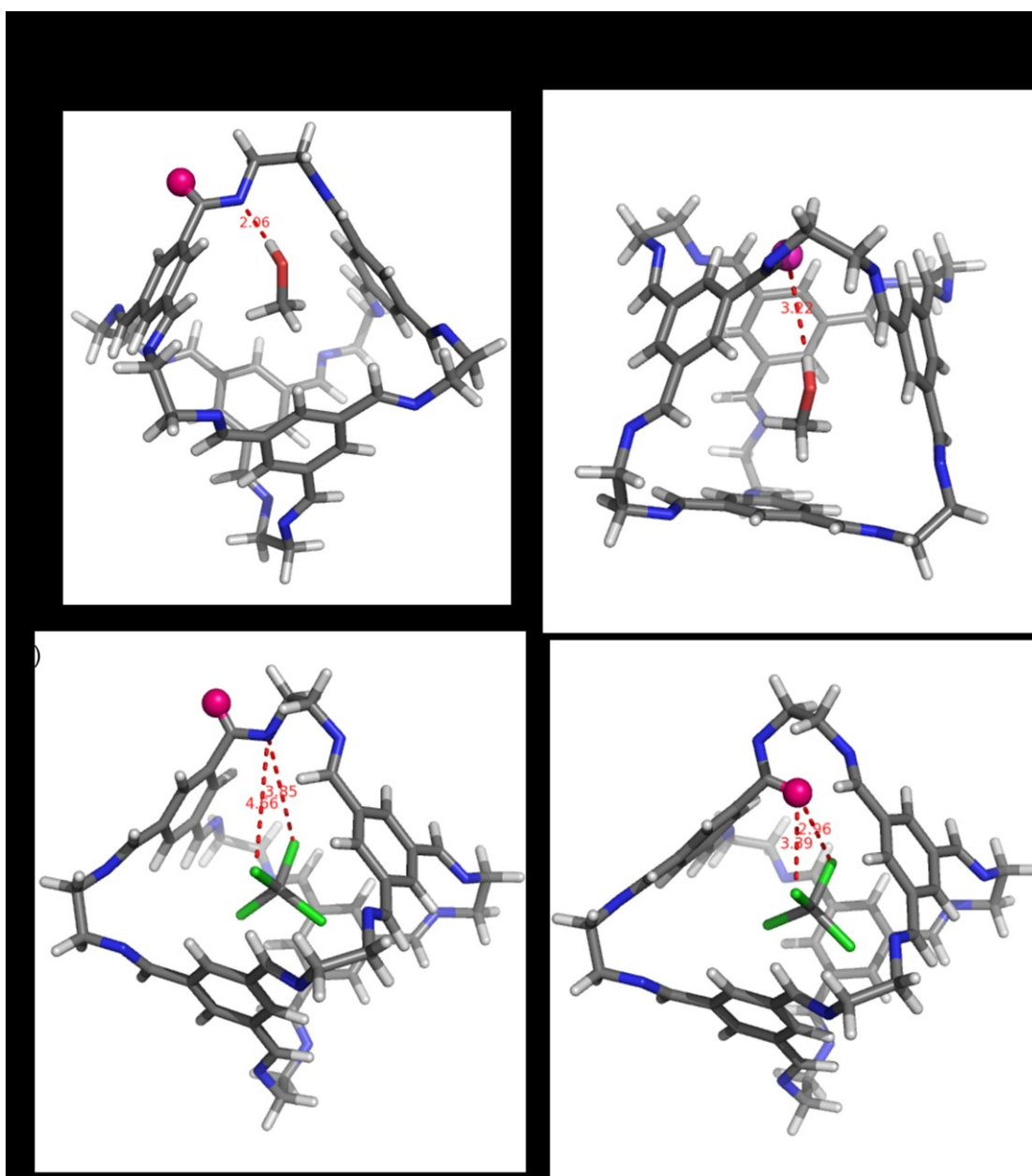


Figure S11 The solvate transition states structures for the “H outside” (left) and “H inside” (right) pathways, with key solvent interactions or close contact distances shown; (a) DCM inside cage (b) external DCM molecules (only key molecules shown for clarity) (c) EtOAc (d) MeOH and (e) CCl₄.

Coordinates of key structures

“TS outside” gas phase, single rotation from 1-T_d-R

E = -419.412026326011 Ha

N	7.2600267367	13.4322783316	6.0595070360	C	12.3822043623	9.5969967566	14.0522846104
N	9.9987669551	13.0878243763	4.9574597247	C	11.9449384432	5.9254751678	8.2412088168
N	8.5056115599	13.4613862772	13.4812020231	C	6.9367922826	15.0474896493	12.4377542030
N	5.8725024094	5.7034065762	9.0077486936	C	16.5081189833	13.2091412874	9.4328193656
N	4.3076178999	8.0975478977	8.3133739889	C	11.8202978539	7.6261111234	15.2266945961
N	15.3306286075	13.0124127740	8.5854970771	C	13.1881177695	5.2818516309	6.3341642322
N	15.2007348338	13.2594710314	11.5221869902	H	7.4908558299	12.9174356526	3.9866503622
N	10.7012389365	6.6037033843	13.2729631864	H	7.0181898793	14.6019464156	4.3546930777
N	6.7038496103	14.2773515297	11.2087772390	H	5.6071903286	9.9242067139	6.9545222155
N	13.4137646922	7.6363224313	5.6895203453	H	10.7871037040	10.5917550236	5.1869317373
N	11.5938443994	9.0244847750	14.8804863229	H	11.6518368366	14.6785562704	12.4787720250
N	11.9311605764	5.4214022295	7.0645164956	H	7.4009005737	6.3782365010	11.0658902932
C	6.3954603902	11.8215223442	7.6500122916	H	9.2576061471	15.0734930952	5.3105535415
C	11.7497720042	12.1398042833	6.3358695615	H	9.3393782177	14.5301385457	3.6101754253
C	10.8605438775	13.0360026236	13.6509009707	H	5.4319896043	10.5514385319	11.1988904842
C	8.2648269098	6.0660179465	9.1160595862	H	14.3871381989	9.4179518127	7.2327847220
C	5.7936292711	10.5655096015	7.8124039453	H	14.0362787347	11.1011775610	12.5062182438
C	11.6248556492	10.8235583795	5.8398843035	H	11.7053247201	6.4452429170	10.9017249623
C	11.8117681764	13.6566050457	12.8161602210	H	6.5112868813	13.6356546572	14.0606456891
C	8.3295203741	6.3055458679	10.5054389268	H	7.4907692262	15.0430820058	14.5356080731
C	5.4235680331	10.1044774445	9.0888536571	H	7.0593729327	13.6166169084	8.6523141014
C	12.5743686282	9.8478880511	6.1583059040	H	12.9491175983	13.4612637427	7.5610169335
C	12.9631617969	12.9628831712	12.4077447328	H	10.3187690093	11.2273096934	14.6806100156
C	9.5650027415	6.4387609238	11.1481695122	H	9.4263131402	5.7910248875	7.3128841181
C	5.6888821306	10.9123533402	10.2035832364	H	4.8566451534	5.7394579191	7.1165715644
C	13.6546552312	10.1858743122	6.9996069231	H	6.6673540754	11.5148185985	5.4974623345
C	13.1403304247	11.6291733384	12.8240251158	H	10.8583171044	14.1325555039	6.5431246180
C	10.7522828174	6.3421437135	10.3903560953	H	9.7135693033	14.6331069865	14.7124797480
C	6.2534972465	12.1932529729	10.0553557417	H	7.0392575778	5.9916121178	7.3073427217
C	13.7959645450	11.4817764991	7.4997382861	H	4.1471979077	4.7023278215	8.3899996773
C	12.1914821093	11.0003273334	13.6382903482	H	4.6605016508	8.4730383576	10.3312118226
C	10.7014712449	6.0958307037	9.0168496178	H	11.5177276837	8.2555313124	5.0720263704
C	6.6068113323	12.6389877986	8.7758757220	H	13.6623564920	14.6109010472	11.1428364639
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C	11.0547739923	11.7222826885	14.0554606949	H	3.4929132540	6.6895044541	9.7146378749
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C	6.7974965075	12.2640777841	6.2993378295	H	12.3059477347	6.1821221109	4.5538556780
C	10.8018891904	13.2050671554	5.9463928184	H	14.0902591413	6.0472370946	4.5260701675
C	9.6192130582	13.7833056353	14.0163803354	H	15.6999202660	14.9980020981	10.3656826003
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C	7.6407122658	13.7586919388	4.6865556445	H	9.6926859469	7.1824541831	15.0782367568
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C	7.3281886055	14.2948257159	13.7375854698	H	6.4306126618	12.4557155427	12.2036247114
C	4.6557623968	5.6571983176	8.1990236162	H	15.5459112411	10.9435009732	8.6969007155
C	4.7608922767	8.8025102744	9.2817819296	H	13.2502071020	9.0746945034	13.6133467191
C	12.4626638167	8.4873130853	5.5938392481	H	12.8817930267	6.2191247606	8.7450450633
C	13.9923977984	13.6713828036	11.6208858629	H	7.7375150000	15.7632508352	12.2061028063
C	9.6093246832	6.6481905287	12.6082345543	H	6.0360387906	15.6515089230	12.6267795108
C	3.7087040833	6.8023515139	8.6378552007	H	16.9740021602	12.2580090743	9.7443204789
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C	16.1223364005	14.0299169992	10.6872475307	H	12.7638392049	7.2241268516	14.8161978301
C	10.6481380642	6.7589277574	14.7232610398	H	11.8571592360	7.5507401631	16.3223748005
C	6.4742986879	13.0196429940	11.2613248556	H	14.0786372334	5.4396796269	6.9669043514
C	14.9710742518	11.8113919360	8.3274498781	H	13.2271280321	4.2662550600	5.9187484536

“TS inside” gas phase, single rotation from 1-T_d-R

E = -419.411627167476 Ha

N	7.0915305613	13.2731483467	6.1672217199	C	12.2871491921	9.5614809270	13.6452948382
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N	8.7422903307	13.8911779069	13.5822854379	C	6.8056487521	15.0516746725	12.2794435415
N	5.7644959595	5.6017138847	8.9656508349	C	16.6731873110	13.1923600692	9.2264159908
N	4.1214428760	7.9233087817	8.3416274136	C	11.7084226916	7.6896693222	14.9566936648
N	15.5026355828	12.9902310668	8.3726502910	C	13.0948168494	5.1757499338	6.1369736951
N	15.2792479216	13.1844425168	11.2561239120	H	7.4695351017	12.7658757053	4.1134528864
N	10.6600779265	6.4361636042	13.1054389952	H	6.9210187902	14.4330686476	4.4523813665
N	6.5303993461	14.1600638541	11.1451574415	H	5.4731298480	9.7355674291	7.0359917199
N	13.4476838714	7.5598832739	5.6104593260	H	10.8218404638	10.5343503915	5.1951059852
N	11.4132865216	9.0059094289	14.3959041780	H	11.5422223411	14.4557549165	11.5845073057
N	11.8148037464	5.3283364101	6.8281516857	H	7.3472189641	6.3258759967	10.9383072155
C	6.2070953703	11.6543893170	7.7333828769	H	9.1050536504	14.9294063745	5.5834239193
C	11.8140030882	12.0800812899	6.3214785053	H	9.2541966125	14.4981925233	3.8568898122
C	10.5982986132	12.7607718328	12.5312404917	H	4.9895241133	10.4763289127	11.2408070521
C	8.1582837920	5.9722595702	8.9753634252	H	14.5274857366	9.3872021357	7.0623265619
C	5.6006480799	10.3998053054	7.8869615135	H	14.1346895069	11.1307632904	12.4222743454
C	11.6898558283	10.7719502580	5.8046943596	H	11.6461414530	6.3256112719	10.6750753556
C	11.6875765316	13.4528903242	11.9812545381	H	6.7257716003	13.7018282514	14.0206518799
C	8.2615558290	6.2385737108	10.3569440579	H	7.3995774561	15.2854882531	14.3260345332
C	5.1411372659	9.9718591691	9.1459536436	H	6.8149776270	13.4630978402	8.7358816789
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C	12.9631912739	12.8704998145	11.9431806799	H	9.9577902103	10.9185477225	13.4605092183
C	9.5123673679	6.3606585954	10.9712978836	H	9.2708871090	5.6552097675	7.1467951411
C	5.3217091147	10.8111757177	10.2586456589	H	4.6768235825	5.5648278142	7.1144818804
C	13.7771170302	10.1481219306	6.8645541197	H	6.6574747181	11.3106970438	5.6117421462
C	13.1434655325	11.5753179462	12.4619430069	H	10.9019821109	14.0502721700	6.6325320038
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C	12.9343384965	12.4067389867	7.0902339410	H	8.6339361807	6.8833213702	12.9098259226
C	10.7889593514	11.4780943142	13.0418122995	H	3.3251329055	6.4931155842	9.7281330755
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C	6.6861506003	12.0829915166	6.4011539037	H	12.3156922595	6.2051649213	4.3864725900
C	10.8115538658	13.1261667888	6.0337989972	H	14.0907348666	5.9924608621	4.4041011909
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C	4.5182091385	5.4989155595	8.2050453546	H	15.7231822629	10.9238142963	8.4997895098
C	4.4839879677	8.6631200317	9.3212923105	H	13.2630131570	9.0877573581	13.4372519764
C	12.5289901696	8.4461908961	5.5042083442	H	12.7699312619	6.0021444826	8.5552009610
C	14.0735918244	13.6106827523	11.2970226985	H	7.4980529433	15.8185758603	11.9076346608
C	9.5849658811	6.5909897203	12.4295389307	H	5.8715089667	15.5823726501	12.5235173389
C	3.5453292937	6.6161382523	8.6532041405	H	17.1542167991	12.2433843621	9.5214291420
C	13.2179560527	6.2430985210	5.0215663031	H	17.4056553561	13.8018084561	8.6797110729
C	16.2503909715	13.9722738910	10.4971592562	H	12.6956305972	7.3021104133	14.6488637241
C	10.6123969037	6.6826249875	14.5485986619	H	11.6956184393	7.7773710603	16.0524773350
C	6.1104305876	12.9623665121	11.2959928954	H	13.9629954877	5.2597997866	6.8132403425
C	15.1398826266	11.7869786206	8.1328934347	H	13.1114421107	4.1842168066	5.6658599773

TS gas phase, combined first and second rotation from 1-T_d-R

E = -419.401738512354 Ha

N	24.061503408	27.554018327	19.584589138	C	26.194782682	20.341563632	22.948439468
N	22.883206955	28.194196084	28.699092759	C	21.012765499	29.389604990	27.428780566
N	20.133130771	20.474609748	23.936376352	C	30.598953932	27.629207676	24.091968031
N	18.359983383	22.890815842	23.403258337	C	26.238145343	21.778455388	29.809026915
N	29.501131677	27.398810046	23.131345504	C	27.344910177	19.780751153	20.924190151
N	29.172500233	27.670656285	26.114863640	C	21.724580804	27.186364001	18.459591726
N	24.977085621	20.532108932	28.076559438	H	21.077555416	28.852807566	18.571710232
N	20.916388951	28.403365543	26.343242107	H	20.050076022	24.429955686	21.858564138
N	27.449852329	22.137878081	20.203436057	H	24.931300120	25.130836760	19.674481735
N	25.854123142	23.123228072	29.341126267	H	25.358981420	28.607435821	26.598412204
N	26.121390789	19.881678410	21.741556877	H	21.763286038	20.971195954	25.938542738
N	20.528602721	26.504054528	22.303425982	H	23.148865970	29.510188847	19.950899779
C	25.914481642	26.656362980	20.843400474	H	23.4705777417	29.064191472	18.249245640
C	24.687555941	26.909997108	27.745811599	H	19.013299524	25.790850842	25.819866878
C	22.543129219	20.648569157	23.951830305	H	28.419647962	23.855474630	21.886204039
C	20.027095403	25.226418055	22.603877853	H	28.300230814	25.530306586	27.320412052
C	25.756894510	25.351655006	20.356139970	H	26.062671614	20.667311346	25.630139898
C	25.637682308	27.646923552	27.030989507	H	20.793274810	27.854095830	28.982751240
C	22.663656179	20.840726156	25.334025594	H	21.444243872	29.415242395	29.560948572
C	19.486792469	24.968666681	23.869393094	H	20.857959392	28.517967025	23.019894042
C	26.658358410	24.344104794	20.738279052	H	27.122533205	27.970821996	22.089126191
C	26.941529232	27.145145295	26.879889073	H	24.288731407	25.115113943	28.897986058
C	23.935274247	20.853980147	25.931356845	H	23.611889438	20.308808322	22.088584059
C	19.428410172	25.988429197	24.832849441	H	18.931969030	20.621672912	22.110719268
C	27.716657453	24.644209787	21.605590573	H	21.638129360	25.833047391	20.548022942
C	27.283437529	25.909939815	27.445271558	H	25.131803423	28.681429334	21.045343361
C	25.082152555	20.670286187	25.149028942	H	22.683818588	26.992881315	26.926393570
C	19.924858054	27.259019012	24.523529641	H	21.292172039	20.800989736	22.175683717
C	27.874302081	25.950451244	22.097123207	H	18.390785167	19.462837600	23.363341112
C	26.324780891	25.172458113	28.161587512	H	19.290262712	23.319483234	25.279228150
C	24.962541001	20.484462415	23.761357848	H	25.418703030	22.741019912	19.922938354
C	20.471288716	27.525866559	23.261401233	H	27.438843205	28.735200415	25.475402270
C	26.979204392	26.955871329	21.711889823	H	23.274204394	21.791378540	27.786923201
C	25.028159899	25.681121449	28.325779075	H	17.834735783	21.398719760	24.911576329
C	23.694677950	20.469042159	23.166548222	H	16.887670864	21.411250233	23.390747141
C	21.150766491	26.728223582	20.973955808	H	26.275609702	20.590745251	19.194915050
C	24.971717109	27.743557964	20.484186996	H	28.056547944	20.537588419	19.004443743
C	23.279687090	27.389653480	27.773615239	H	29.654849233	29.425918623	24.903710434
C	21.227289828	20.649113642	23.268774222	H	30.954772984	28.746419657	25.932027604
C	21.711206929	28.099677223	19.096993325	H	24.138155745	21.196424442	29.981048242
C	23.144915834	28.656232414	19.236321858	H	25.290223205	19.823933416	30.015770463
C	21.489990000	28.681340622	28.719926023	H	18.977406272	28.933076628	25.574838262
C	18.847211784	20.469859207	23.210903688	H	29.293457640	25.332288923	23.631076359
C	19.017947597	23.612223552	24.249202715	H	27.741642234	23.538064982	28.434439951
C	26.453829180	22.962532865	20.236294597	H	27.117564902	20.662409465	23.462627876
C	27.906441247	27.936091629	26.079232244	H	21.773078759	30.150063831	27.123426519
C	24.040331961	21.101743465	27.391344045	H	20.075179016	29.946534526	27.641465225
C	17.912734648	21.543051109	23.810278354	H	31.081719542	26.700479333	24.471781589
C	27.237811090	20.756641846	19.729857591	H	31.384610852	28.203784473	23.546391927
C	30.090231413	28.473771501	25.282092692	H	27.176425359	21.380234243	29.361394789
C	25.074355731	20.802087035	29.525479353	H	26.402274608	21.835405238	30.911031303
C	19.890985993	28.320662727	25.569845568	H	28.293054355	19.966704034	21.477008084
C	28.983438940	26.216709699	23.045242514	H	27.392531882	18.735262707	20.538262737
C	26.707488327	23.837156401	28.681561929	H	27.376175345	18.711506833	20.504379605

“TS outside” one DCM molecule, lowest energy, first rotation from 1-T_d-R

E = -456.169205361685 Ha

N	7.1826070412	13.4581112578	6.0505103714	C	16.2862469503	13.1837816530	9.6679473501
N	9.9461757979	12.8197612574	4.9629337315	C	12.3583666363	6.9716356284	15.4081936795
N	8.9402540508	13.9542713188	13.8556718219	C	13.2149070505	5.0574451224	6.2662457515
N	6.1507657649	5.7905350687	9.6400659495	H	7.4291687882	12.6760576897	4.0677951509
N	4.5827598002	8.2250297466	8.9181234962	H	7.0372211304	14.4130267808	4.2082423661
N	15.1497276716	12.9380771727	8.7803829916	H	5.9328629510	9.9504873284	7.4008071344
N	14.9640672072	12.9365729079	11.7320554559	H	10.8586116832	10.3778992282	5.1894596159
N	11.3409220650	5.7965426883	13.4856458110	H	11.2616125175	13.9747252532	12.7014591778
N	7.0059960032	14.1123261997	11.7083305417	H	7.9052898688	6.1625336442	11.5496313137
N	13.4813103712	7.4625408195	5.7898523817	H	9.3007535384	14.8572740338	5.1787217294
N	11.8616420820	8.2954802171	15.0365081980	H	9.3353448865	14.1882302346	3.5231881886
N	12.0053258327	5.2305721684	7.0689457320	H	5.0599315812	11.2306352686	11.4041433636
C	6.3601166775	12.0281902090	7.8245458037	H	14.3787038795	9.3006839648	7.4209911952
C	11.7451606100	11.9635091244	6.3461126554	H	14.0982076753	10.7443992369	12.8625683009
C	10.5723361287	12.1810912488	13.6692556249	H	12.1619349833	5.8378268179	10.9923882400
C	8.5624417593	5.9656964897	9.5091746093	H	6.9031037576	13.5392720662	14.3895130188
C	5.9246750295	10.7399374926	8.1478791079	H	7.5624998958	15.1163536939	14.9063467208
C	11.6630811675	10.6364146055	5.8734273200	H	6.6958903042	14.0280216415	8.5646265973
C	11.5325613441	12.9664132879	13.0027010387	H	12.8646350444	13.3282662166	7.6025530034
C	8.7707734905	6.0638892000	10.8999306517	H	10.1673325634	10.2442753856	14.5440330049
C	5.4257865008	10.4416553474	9.4299008040	H	9.5321145078	5.7555095042	7.5858401691
C	12.6127104950	9.6803041144	6.2495232314	H	4.9661526567	5.7924409134	7.8487165000
C	12.7982987454	12.4520860904	12.7098924516	H	6.8199228285	11.4265766008	5.7718746797
C	10.6068701443	6.0116866530	11.4354393407	H	10.9001726632	13.9790039391	6.4067530880
C	5.4154271259	11.4528469323	10.4000158526	H	8.4733365250	11.9610277105	14.2541073958
C	13.6448430111	10.0499910296	7.1358480904	H	7.1573387335	6.0248216228	7.8320818277
C	13.1116109876	11.1347401374	13.0993822299	H	4.3371005728	4.8504038772	9.2321297160
C	11.1635529199	5.8808352017	10.5648301883	H	4.6989660802	8.9596184837	10.8617602007
C	5.8653534468	12.7470497961	10.0943658451	H	11.6226674154	8.1010798646	5.1027606108
C	13.7390366755	11.3591300778	7.6165971711	H	13.3717325059	14.2748393081	11.6514667902
C	12.1761930115	10.3454811337	13.7766479634	H	9.3232932085	6.3096445827	13.4726218034
C	10.9742718878	5.7845744644	9.1829000091	H	3.8854991609	6.9478500689	10.4960192413
C	6.3357380949	13.0348784661	8.8131876379	H	3.0078656384	6.8667256346	8.9412802668
C	12.7777460317	12.3144999722	7.2219877909	H	12.3743745007	6.1025808874	4.5512532444
C	10.8961105871	10.8736534255	14.0418306906	H	14.1547238421	5.9387796003	4.5358579696
C	9.6656041697	5.8396953901	8.6611226379	H	15.2938126764	14.8048990344	10.7284463626
C	6.8209773512	12.2980879365	6.4495832083	H	16.6937031317	14.0910373521	11.5790698272
C	10.7993638455	13.0031196501	5.8996946850	H	10.3762625995	6.0747409214	15.3839657562
C	9.2265066754	12.7112281980	13.9555697924	H	11.7332039039	4.9119402930	15.3325555956
C	7.2062569741	5.9407091254	8.9322716381	H	4.9267160669	14.1587216472	11.5354883697
C	7.6111327929	13.5910222888	4.6579112084	H	15.4718110525	10.8810279023	8.8673643171
C	9.1083454507	13.9540826607	4.5732693386	H	13.5229014912	8.6210009049	13.8244816691
C	7.5634385086	14.3760724842	14.0940386008	H	13.1264830729	5.7109763498	8.7606278693
C	4.8627065648	5.7728110866	8.9481357550	H	7.6456795615	15.8987437265	12.5633766599
C	4.8773340891	9.1185003810	9.7835742857	H	5.9822808658	15.4485443048	13.0475623775
C	12.5407422663	8.3232844715	5.6745630945	H	16.8389079950	12.2610599960	9.9185519221
C	13.7607489955	13.2948767180	11.9800673882	H	16.9729827219	13.8742094787	9.1590317215
C	10.2330619858	6.0578866297	12.8997641847	H	13.3580150548	6.7570418236	14.9910530283
C	4.0020159414	6.9718396805	9.3983289565	H	12.4228241806	6.9285280085	16.5042818660
C	13.2854939587	6.1510029328	5.1731558096	H	14.1387193529	5.0907921078	6.8704102993
C	15.8072093087	13.8579928989	10.9725184084	H	13.1576964172	4.0799906896	5.7682805261
C	11.3709644792	5.8755458848	14.9475509683	Cl	8.6931432541	9.8071796317	11.4840974900
C	5.8994107271	13.7699298544	11.1783500563	C	9.0137740784	11.3182659578	10.5275763345
C	14.8664847002	11.7247190468	8.4913386398	H	8.3272298104	11.3099792994	9.6865457117
C	12.5610822577	8.9920047494	14.2211850057	H	8.8529323353	12.1763784468	11.1788298188
C	12.1345227900	5.5779851485	8.2943827441	Cl	10.6912412351	11.3911226781	9.8660043229
C	6.9927291675	15.0578090627	12.8282745809				

“TS inside” one DCM molecule, lowest energy, first rotation from 1-T_d-R

E = -456.165164265515 Ha

N	7.4357069370	13.3929183808	5.9798616602	C	16.3642832373	13.2706879636	9.7360903948
N	10.1524315981	12.9268026368	4.9371646007	C	12.2923647663	7.2126514704	15.4190836835
N	8.9213313501	14.1265206937	13.6757956698	C	13.1872323006	5.1307854926	6.3909436781
N	6.0576524189	5.9145007137	9.5999773370	H	7.6546048743	12.7099067227	3.9559750265
N	4.5026350235	8.3093672850	8.8267026176	H	7.2005448980	14.4250314319	4.1827534925
N	15.2359510066	12.9991250957	8.8462767302	H	5.7235473266	10.0136590700	7.2237996176
N	15.0282801480	13.1752918531	11.7937868741	H	10.8989968234	10.4645837676	5.3023089088
N	11.1797381876	6.1471805701	13.4938327563	H	11.2828020561	14.1780567960	12.6207754474
N	6.3614042881	14.2314980553	11.7093589086	H	7.7696675103	6.4677547270	11.5052025891
N	13.4724582933	7.5198729907	5.8723251905	H	9.4401497958	14.9433723537	5.1157038855
N	11.8800089093	8.5648849860	15.0527680020	H	9.5350941263	14.2606072912	3.4642719497
N	11.9675492172	5.3146965760	7.1689294495	H	5.8585802382	10.9749035474	11.4130862438
C	6.6404687818	11.9131712946	7.7218964450	H	14.4218359045	9.3293723516	7.5096065393
C	11.8409880401	12.0462545556	6.4159848497	H	14.1309675367	10.9558437964	12.8097494200
C	10.6085262142	12.4000499496	13.6339028773	H	12.0387842634	6.1340345130	11.0462745498
C	8.4657157529	6.1477244088	9.4948249560	H	6.9234114614	13.7268183263	14.3589391181
C	5.9983747759	10.7048570243	8.0159893209	H	7.6039827445	15.3301659181	14.7393549796
C	11.7174131984	10.7145841470	5.9721229389	H	7.4939910295	13.7164744356	8.5296827665
C	11.5568841071	13.1752283852	12.9339148607	H	13.0109527863	13.4004725957	7.6265183160
C	8.6490593176	6.3417558719	10.8794098238	H	10.2283433183	10.4854278647	14.5624462905
C	5.6959203581	10.3621137500	9.3468326831	H	9.4719345696	5.8168052554	7.6070964628
C	12.6484513953	9.7423160109	6.3523030107	H	4.8833755980	5.8553539675	7.8044037398
C	12.8228847730	12.6583495653	12.6431873737	H	6.8363420773	11.4358525808	5.5905377247
C	9.9295605987	6.3328964455	11.4387727197	H	10.9551283772	14.0520095162	6.5013669855
C	6.0712264177	11.2387612301	10.3788132012	H	8.5617652165	12.1988299608	14.3860770013
C	13.7038148635	10.0931326332	7.2220744033	H	7.0811306964	6.1166405127	7.7970808716
C	13.1442122716	11.3449196030	13.0479959600	H	4.2539282496	4.9453694181	9.2071947204
C	11.0482383407	6.1534155429	10.5991115415	H	4.9247483926	8.9016972471	10.7754495404
C	6.6866924772	12.4663980396	10.0942538001	H	11.5924642071	8.1698748257	5.2534012251
C	13.8375669892	11.4130610733	7.6730550945	H	13.3877901361	14.4176280497	11.4664486344
C	12.2193526095	10.5699517385	13.7535485873	H	9.1692284709	6.6939396378	13.4632863122
C	10.8845622737	5.9654807397	9.2247660032	H	3.7568680858	7.0638272549	10.4082243612
C	6.9825028125	12.7907550319	8.7712946292	H	2.9132938272	6.9577793332	8.8340318156
C	12.8980798616	12.3829635376	7.2646276197	H	12.3101809757	6.1576050815	4.6873751480
C	10.9455939531	11.1043771252	14.0311149236	H	14.0882365617	5.9719280227	4.6173973206
C	9.5849005975	5.9752383181	8.6763031180	H	15.3743410337	14.9683457196	10.6650578312
C	6.9840774890	12.2467781761	6.3262315277	H	16.7635715286	14.3125107762	11.5817504461
C	10.9152581876	13.0985577476	5.9486842385	H	10.2455936024	6.4739833958	15.3997908544
C	9.2651107567	12.9217206214	13.9367377417	H	11.5064783371	5.2093316296	15.3225319492
C	7.1172717013	6.0662325069	8.8995796112	H	8.2204326141	13.3060846232	11.4277028010
C	7.8113291721	13.6042243735	4.5851704889	H	15.5697167611	10.9418432278	8.9354039074
C	9.2938850697	14.0308694326	4.5119251097	H	13.5241615037	8.8046821077	13.7926149758
C	7.5505133890	14.5483412581	13.9671172793	H	13.0467750863	5.8647026057	8.8650559619
C	4.7719836160	5.8649251996	8.9026850718	H	7.5887176157	15.8720920595	12.2606003139
C	4.9988484376	9.1112817610	9.6932753979	H	6.0173400777	15.7669669972	13.0668209147
C	12.5340400891	8.3850745354	5.7873269600	H	16.8924668936	12.3542991233	10.0542043183
C	13.7937109125	13.4921812867	11.9098413191	H	17.0747194216	13.9094495647	9.1932642050
C	10.0797884185	6.4226283853	12.9023681370	H	13.2684217047	6.9301312805	14.9874855645
C	3.8950973430	7.0730578283	9.3125925630	H	12.3633998189	7.1583443632	16.5144978883
C	13.2411950307	6.2034259757	5.2776474607	H	14.1055998879	5.1899035580	7.0008775548
C	15.8826459487	14.0419109778	10.9846911035	H	13.1453554621	4.1430175815	5.9137588423
C	11.2194065817	6.2045450542	14.9541994052	Cl	10.4622227575	12.9750231021	9.6708992701
C	7.1525754830	13.3752172006	11.1870373509	C	10.9212830849	11.2374413310	9.9034118710
C	14.9642801572	11.7834252428	8.5536859582	H	11.2768487701	10.8664382616	8.9451747474
C	12.5893965943	9.2164570297	14.2116219427	H	11.6836151062	11.2059184298	10.6786329488
C	12.0668334583	5.7102881647	8.3807532309	Cl	9.5446327480	10.1967433736	10.4315934897
C	6.8756737287	15.1777258559	12.7262687670				

“TS inside” 13 DCM molecules, first rotation from 1-T_d-R

E = -897.116664617074 Ha

N	11.8724516092	18.4369593220	11.6784057335	H	9.8174292714	13.9543778604	16.7111895264
N	14.5102478343	17.8434077911	10.4466009153	H	16.0749669269	13.1022656599	11.0890854210
N	13.2808556643	19.1063467934	19.6505768866	H	17.5965738997	19.4727814873	17.0866290702
N	11.1128476877	10.7978892820	15.1441656387	H	14.1779440838	11.6446820237	19.7229093579
N	9.3332837338	13.3944952434	14.7574870361	H	8.8921205941	11.8950773893	16.2327717892
N	19.4751723656	18.2568382968	14.4820779951	H	7.8893351153	11.8999639032	14.7505767904
N	19.3407238808	18.4041637984	17.4657108183	H	16.8295950721	11.0623877851	10.7135852386
N	16.1584613723	11.0094262170	19.7057411398	H	18.6132522806	10.9898765528	10.6415830568
N	10.8133087444	18.7133748134	18.1153483847	H	19.5492604185	20.2227422662	16.3459214223
N	17.9078457096	12.5136734056	11.8718753280	H	21.0010126468	19.6423274972	17.1929936827
N	16.5685654165	13.6636114537	20.950561506	H	15.3022669296	11.3481599532	21.6452088828
N	16.6230573909	10.2747974787	13.2862559312	H	16.7606089299	10.3178416461	21.5827931049
C	11.2153983670	17.0455558593	13.5628390429	H	11.6536146522	19.7598854631	16.5286833842
C	16.1535878344	17.0365013397	12.0374620557	H	19.9021931481	16.2257032198	14.6288967068
C	15.0703854585	17.4697478583	19.5487711070	H	18.2293036930	14.0911377317	19.7810942953
C	13.3339401879	11.4097523515	15.7858649539	H	17.8242420674	10.7254795793	14.9295488167
C	10.7153378815	15.7901591487	13.9241114590	H	11.4220965314	20.7372459258	18.4720390589
C	16.0786110235	15.6745883536	11.6819813494	H	10.0467507073	20.1384259483	19.4324410761
C	15.9174730714	18.2157858330	18.7052708563	H	21.1956260723	17.7078728621	15.6371302374
C	13.5721639429	11.5030734393	17.1621888375	H	21.2614521752	19.2850870438	14.8022676806
C	10.3537615067	15.5121790240	15.2572989356	H	18.1804665908	12.2431553680	20.9738933172
C	17.0357968395	14.7627932813	12.1412830587	H	17.3215262616	12.5021876519	22.5149697792
C	17.1851267356	17.7350495906	18.3519946247	H	18.7372179721	10.1445324299	12.9612181780
C	14.8570664583	11.2758297766	17.6815394566	H	17.7042345070	9.1127220511	11.9323417646
C	10.5384882276	16.4929725179	16.2321637339	Cl	14.2483181794	15.1820594533	15.0595840691
C	18.0649055280	15.2203494835	12.9897334184	C	14.5925912810	14.9023298420	16.8112012434
C	17.5834920030	16.4569487845	18.7984342772	H	15.0667267661	13.9279254325	16.9103389259
C	15.9184765043	11.0119297894	16.7971051274	H	15.2190091237	15.7161668273	17.1686935900
C	11.0409103317	17.7635600646	15.8914655747	Cl	13.0936247094	14.8854826992	17.8304237421
C	18.1430656946	16.5650384391	13.3690955346	Cl	21.0387254515	14.9658655377	17.2370249967
C	16.7560903442	15.6999200614	19.6394237083	C	21.3631365238	16.1035245642	18.6122307104
C	15.6942032844	10.9269938113	15.4179439156	H	22.4317838583	16.3083669497	18.6247239253
C	11.3771795601	18.0304901573	14.5596188963	H	20.7437700783	16.9870757520	18.4378575722
C	17.1702099347	17.4647708314	12.8944468632	Cl	20.9232513231	15.4062085313	20.2252630855
C	15.5090653333	16.2294764224	20.0223705598	Cl	11.1850752851	6.8520148238	16.4171979292
C	14.3951319054	11.1473752644	14.9204848151	C	11.1665823498	8.3854758908	17.3803677907
C	11.5339557795	17.2917927322	12.1446682733	H	11.2751982730	9.2137895273	16.6753282486
C	15.2283166561	18.043823350	11.4876824548	H	10.2281745865	8.4135238172	17.9323101624
C	13.7472888204	17.9601931759	19.9796198658	Cl	12.5109956295	8.4810370136	18.5945349190
C	11.9995894191	11.7187027077	15.1874159949	Cl	21.6418814621	13.9048867440	13.6311849602
C	12.1466220413	18.5302221575	10.2410489570	C	20.9011235218	12.3140630164	13.1635727298
C	13.6252874343	18.9154932071	9.9936746570	H	21.0635819047	11.6274149305	13.9925320667
C	11.9596937012	19.4789464330	20.1657101515	H	19.8479466234	12.4847697428	12.9294633840
C	9.8209564833	11.0039463967	14.4598353975	Cl	21.65166561574	11.5858254068	11.6888331497
C	9.7976170418	14.2008267741	15.6374966762	Cl	12.7341718346	22.4589256624	11.5708651815
C	16.9704083347	13.3640489346	11.6697050421	H	12.6362346271	20.3431826653	12.6499717086
C	18.0785375734	18.6068772265	17.5648574682	H	14.2025616850	21.2147990296	12.9679354235
C	15.0523934800	11.3234543092	19.1397328039	C	13.1201551521	21.2911978536	12.8957339454
C	8.9037271772	12.0531301662	15.1403312952	Cl	12.5238108824	21.8375261726	14.5232099366
C	17.7540317979	11.1702708757	11.3005328284	Cl	13.1997487300	23.0225756776	18.2233227147
C	20.1159102387	19.3225694252	16.6269629344	H	14.0235608185	20.7929898783	18.2942137302
C	16.2766823763	11.2035919772	21.1521568713	H	14.4548793153	21.6573289740	16.7409581575
C	11.1980640753	18.8278576650	16.8981815045	C	14.3855917267	21.7107798533	17.8253683176
C	19.2550592429	17.0187846227	14.2266108256	Cl	16.0464480419	22.0350090235	18.4688792795
C	17.2317709162	14.3917109205	20.1368398364	Cl	19.4900408336	9.5960154515	17.3374681168
C	16.8126940662	10.6306810113	14.5014491064	H	17.7529633505	9.6644322395	18.9845512623
C	11.0195396389	19.8608701805	19.0030837667	H	18.5755480937	8.0344294194	18.8823830215
C	20.6066397565	18.5941505669	15.3508939325	C	18.6941321927	9.1160395692	18.8996067052
C	17.1925146037	12.4199491521	21.4271516193	Cl	19.6841729048	9.5453646125	20.3518519741
C	17.7806758060	10.0959321251	12.4137374627	Cl	12.9331402159	15.0156712716	22.7843472339
H	11.9210660284	17.5917004868	9.7098840606	H	12.6771847883	14.1163556706	20.6057843997
H	11.5198706509	19.3310855562	9.8267009801	H	14.2388235442	13.6078269715	21.3806454394
H	10.6129611549	15.0084376164	13.1774777292	C	13.1646107132	13.7557239553	21.5082886835
H	15.2711280891	15.3374136830	11.0422246280	Cl	12.4125944015	12.1631931366	21.9300545003
H	15.5979021397	19.1922247083	18.3636017420	Cl	9.4627285855	16.9573506800	21.7362165893
H	12.7513666663	11.7234210406	17.8376064230	H	8.2327602451	16.3937224164	19.7827093943
H	13.8418642829	19.8806093672	10.4782620422	H	9.8395975600	17.1491051406	19.3842136081
H	13.7639747367	19.0405114342	8.9114840839	C	9.2946176628	16.4434580142	20.0174477101
H	10.2946300814	16.2807985500	17.2654285424	Cl	9.9800758800	14.7788212775	19.7115659237
H	18.8141418222	14.5187807141	13.3386800952	Cl	16.3321997511	20.7412129418	14.6877097108
H	18.5447059994	16.0640982078	18.4878809240	H	18.5460401946	20.2329161633	13.9845789677
H	16.9184240795	10.8693755937	17.1919610184	H	17.7348670367	21.4575845805	12.8985763159
H	11.5058156867	18.6819255421	20.7739065568	C	17.9408687024	21.1416764469	13.9195781691
H	12.0843874855	20.3673309767	20.8000455593	Cl	18.7980402300	22.4832447754	14.7578036882
H	11.7557597231	19.0087999343	14.2853147885	H	15.6947991547	14.1888319878	8.2540011355
H	17.2216327393	18.5027265832	13.1981115904	C	14.3013828635	15.3358672097	8.3730952540
H	14.8867746159	15.6637818893	20.7033662085	H	14.6214373616	16.2207078694	8.9277375325
H	14.2310556213	11.1479909794	13.8495070292	H	13.9628767939	15.5512621313	7.3614399886
H	9.9774082203	11.2998125843	13.4151607758	Cl	12.8918077676	14.6472495564	9.2865114459
H	11.4430648624	16.4139222522	11.4851532096	Cl	14.8105180297	8.7324076514	10.0836965717
H	15.2214607385	19.0138731092	12.0137505225	C	14.0281984664	9.6019799904	11.4660356289
H	13.1804088087	17.2731684141	20.6280868555	H	13.1023036232	9.0847423291	11.7096988124
H	11.8996099665	12.6888385181	14.6814259237	H	14.7564623802	9.6352726531	12.2787526646
H	9.3026969348	10.0394546882	14.4592633757	Cl	13.6081343712	11.3222436162	11.0648429428

Cl	7.3861814402	11.9987174816	11.6567027333	H	8.5896903790	13.7792157761	12.6712761100
C	8.4885003006	13.4371259365	11.6402934206	Cl	10.1584089984	13.0281709458	11.0670479722
H	8.0670803330	14.1718254649	10.9568232296				

“TS outside” one MeOH molecule, first rotation from 1-T_d-R

E = -443.489916708019 Ha

N	7.1830423938	13.4984094785	5.8678746636	C	12.3165244791	7.0820547120	15.4108978186
N	10.0300049902	13.0417138713	4.9489971008	C	13.2085271868	5.2618034832	6.3987901507
N	8.9514609682	14.0363194292	13.9418469747	H	7.5876579380	12.7393435844	3.8988032365
N	6.0545283864	5.9603005413	9.5654904323	H	7.0762746760	14.4477233407	4.0199136710
N	4.4766337988	8.3293191707	8.7395135654	H	5.7280581036	10.0331907393	7.1873916659
N	15.2226499975	13.1694422182	8.7643783910	H	10.9062361629	10.6276943970	5.1914680172
N	14.9720653791	13.0998033696	11.7202684102	H	11.2817594695	14.1048624317	12.7780136621
N	11.1674974356	5.9732650829	13.5312823798	H	7.7486456891	6.3577425717	11.5336812548
N	6.7825536422	13.7118206647	11.9901686128	H	9.2395637981	15.0312167609	5.1391306482
N	13.4670086267	7.6641895067	5.8905356212	H	9.4293158908	14.3838960063	3.4854388281
N	11.8925366318	8.4326796562	15.0503903676	H	5.1086482458	11.3228159471	11.2389269225
N	11.9798185583	5.4249740035	7.1686607055	H	14.4088616142	9.5238554244	7.4376101971
C	6.3039919210	12.0777095649	7.6142174027	H	14.1458811544	10.8870880799	12.8538140203
C	11.7899966088	12.2019227309	6.3660907937	H	12.0187415442	6.0199713554	11.0950919594
C	10.6316492255	12.3058648150	13.7668351501	H	6.9875842799	13.5859373282	14.6953700187
C	8.4656764229	6.1480839904	9.5119520740	H	7.5730440828	15.2572914392	14.9290058191
C	5.7877605354	10.8172463491	7.9379129993	H	6.7550587309	14.0538503749	8.3385537807
C	11.7077446043	10.8781658805	5.8813011429	H	12.9183420149	13.5586570901	7.6201320909
C	11.5643726799	13.0947481282	13.0628564388	H	10.2693358923	10.3730403581	14.6598720680
C	8.6328872860	6.2544409929	10.9100196785	H	9.4846017505	5.9164997621	7.6181069923
C	5.3270319124	10.5412271786	9.2388705392	H	4.9254307199	5.8743090863	7.7416518008
C	12.6460484057	9.9145683581	6.2629851080	H	6.7789674280	11.4763944043	5.5598188469
C	12.8242870573	12.5858000895	12.7288214858	H	10.8855703509	14.2059924731	6.4592723561
C	9.9076807160	6.2035683753	11.4812867520	H	8.5971539384	12.0643068123	14.5206911480
C	5.4184307850	11.5376504370	10.2210550263	H	7.1175367711	6.1708975947	7.7862373296
C	13.6789839384	10.2776641750	7.1538849929	H	4.2776268673	4.9626370765	9.1358572876
C	13.1619853467	11.2693210809	13.1137170285	H	4.5444969330	9.0915412125	10.6765881469
C	11.0329532795	6.0631375205	10.6394166926	H	11.6683828781	8.3437527162	5.0868965447
C	5.9619010691	12.7969170880	9.9137136212	H	13.3718555765	14.4312649814	11.6907950862
C	13.7865033247	11.5881080982	7.6285063310	H	9.1589223592	6.5365630593	13.5177961907
C	12.2529898316	10.4814321421	13.8270325944	H	3.7175189736	7.0779024732	10.3111622999
C	10.8840815660	5.9568126073	9.2540625878	H	2.9181507008	6.9489777498	8.7171017918
C	6.3598431444	13.0776182371	8.6061035399	H	12.3797122092	6.2797725345	4.6616709160
C	12.8237562168	12.5443094062	7.2415191651	H	14.1608796379	6.1279527725	4.6675747182
C	10.9791185113	11.0039457296	14.1324418923	H	15.2811750245	14.9871823278	10.7448163410
C	9.5901783331	6.0086013692	8.6958260221	H	16.6774183780	14.2913061404	11.6152138957
C	6.7852251654	12.3427362718	6.2443752041	H	10.2728816522	6.3359831268	15.4493034931
C	10.8336737594	13.2405370291	5.9255969985	H	11.5364995822	5.0735900253	15.3704386875
C	9.2937695332	12.8149315692	14.1180766447	H	5.5642936410	14.8178110897	10.7125790523
C	7.1297668591	6.1107479402	8.8887177237	H	15.5215352844	11.1100025551	8.8780070439
C	7.6737762659	13.6607156232	4.5009497992	H	13.5832751463	8.7324208044	13.8647130285
C	9.1476438007	14.1242349201	4.5160526330	H	13.0487268541	5.8617503404	8.9049149257
C	7.5672948376	14.4056895726	14.2342421522	H	7.5017066801	15.6348006138	12.4670787369
C	4.7880921596	5.8886128973	8.8371821968	H	5.8948942465	15.2730371509	13.1477991872
C	4.7486886400	9.2343128817	9.6014744056	H	16.8981809543	12.4919204098	9.9229384896
C	12.5618700807	8.5502531283	5.7022543525	H	17.0247104359	14.1252385290	9.2051810613
C	13.7699281903	13.4457863755	11.9917507918	H	13.2844913563	6.7987880222	14.9612042608
C	10.0628222643	6.2556876160	12.9495186559	H	12.4140451942	7.0384283906	16.5047157886
C	3.8866078487	7.0803527200	9.2199779031	H	14.1183198114	5.3169392963	7.0221362859
C	13.2832279518	6.3424446082	5.2933658051	H	13.1781228726	4.2776614855	5.9115500846
C	15.8100388381	14.0479267418	10.9852035106	C	8.3954722236	10.2292072698	11.5089046421
C	11.2370107013	6.0594760168	14.9880155558	H	8.4584150351	9.1587109879	11.7273213387
C	6.0635144692	13.8607999749	10.9453616302	H	9.4009534891	10.6635208918	11.6066506056
C	14.9262196622	11.9551312892	8.4898393827	H	8.0503466258	10.3528079465	10.4714954088
C	12.6266525529	9.1194923658	14.2583602711	O	7.4662600634	10.8020220710	12.4552580954
C	12.0719604993	5.7475022548	8.4031477451	H	7.3860146943	11.7680883252	12.2762056796
C	6.8875188780	14.8505934193	12.9303573518				
C	16.3373309207	13.4111452576	9.6789772135				

“TS inside” one MeOH molecule, first rotation from 1-T_d-R

E = -443.484549118587 Ha

N	7.4280545847	13.3917155202	5.9701943950	C	16.3427086451	13.3325242091	9.7682199902
N	10.1536196607	13.0186887882	4.9426535746	C	12.3147603918	7.1298282662	15.3710145804
N	8.8397920032	14.0940090798	13.7441433421	C	13.1316260640	5.1546122089	6.4214186777
N	5.9623011284	5.8077461755	9.6986504912	H	7.6879778321	12.7344111245	3.9415327288
N	4.5901419684	8.3519641709	8.9245043786	H	7.1647459370	14.4278435575	4.1814540450
N	15.2196124709	13.0881736930	8.8636915635	H	5.8190356840	9.9862903713	7.2984351506
N	14.9688402304	13.1232930239	11.8096645413	H	10.9127697697	10.5385280355	5.2783652235
N	11.1699593453	5.9416797827	13.5580890628	H	11.2417837616	14.1684560727	12.7245695730
N	6.2635992956	13.9487331405	12.0122862378	H	7.6930939680	6.0390279209	11.6226963929
N	13.4497436580	7.5628405532	5.9741329381	H	9.3787937473	15.0116450855	5.1575872532
N	11.8292785328	8.4680830579	15.0262337664	H	9.5173142276	14.3684935583	3.4929472722
N	11.8931531954	5.3169585248	7.1798632046	H	5.8534186830	11.1331331677	11.4492158220
C	6.7223233455	11.9081904505	7.7323548163	H	14.4150651657	9.4387277931	7.5272989735
C	11.7852274674	12.1079446970	6.4659278666	H	14.0790504616	10.9349191586	12.8821268957
C	10.5672374739	12.3891745468	13.7364944546	H	11.9638202435	5.8641642571	11.1120894096
C	8.3793275506	5.8791861819	9.5890261207	H	6.9188300253	13.7032541372	14.6276185206
C	6.0800847712	10.7102160774	8.0658773624	H	7.5898318133	15.3441991941	14.8371081060
C	11.7099652572	10.7885598964	5.9735288989	H	7.5702500765	13.7366542531	8.4826583559
C	11.5132426451	13.1596349989	13.0250701901	H	12.9012196956	13.4655257459	7.7296317420
C	8.5693333860	5.9697018484	10.9840813306	H	10.1783141070	10.4714683415	14.6531268284
C	5.7562737083	10.4211579992	9.4066281685	H	9.3759414361	5.7074766761	7.6755912891
C	12.6494088913	9.8255550184	6.3563210866	H	4.7815143104	5.8610713741	7.9068549637
C	12.7772545436	12.6415310222	12.7241950137	H	6.9652972686	11.3877567448	5.6099702113
C	9.8545680736	5.9689333246	11.5327698057	H	10.8005430072	14.0688085328	6.6271696020
C	6.0838748728	11.3457132630	10.4095148357	H	8.5741229266	12.2201248066	14.6192970515
C	13.6819920360	10.1906613155	7.2465842833	H	6.9946253962	5.9438461584	7.8942605855
C	13.0951259175	11.3277479388	13.1250213158	H	4.0753484175	5.0104098178	9.3124293756
C	10.9694530111	5.8725003279	10.6735527939	H	4.9327530323	9.0179425905	10.8677900259
C	6.7038759129	12.5655133367	10.0810932084	H	11.6705287198	8.2763409864	5.1611022097
C	13.7858436813	11.5015686833	7.7247174303	H	13.3712263517	14.4498135704	11.6406347000
C	12.1702680821	10.5496671816	13.8295623332	H	9.1051655862	6.2256392876	13.5787268269
C	10.7987012138	5.7664518775	9.2908590875	H	3.7939428454	7.1621225535	10.5231144533
C	7.0537191531	12.8200605836	8.7540064011	H	2.9140123884	7.1167064308	8.9688161637
C	12.8143884931	12.4519858522	7.3468161783	H	12.3501925190	6.2290016457	4.6982634081
C	10.9007478126	11.0878001080	14.1269756567	H	14.1280241579	6.0382658663	4.7257496671
C	9.4948064102	5.7841234155	8.7531360705	H	15.3463391428	14.9766945153	10.7931767405
C	7.0590416945	12.2203721357	6.3293219009	H	16.7173664870	14.2521060114	11.6821514206
C	10.8344503389	13.1485571900	6.0180136617	H	10.2973461406	6.3158479356	15.4856026688
C	9.2277976847	12.9171970598	14.0726608373	H	11.6037713352	5.0978026147	15.4083583485
C	7.0288809258	5.8796892091	8.9960299424	H	8.0569547515	14.0623017255	10.9529670506
C	7.8033970979	13.6275880562	4.5803956527	H	15.5292857030	11.0304989592	8.9658032147
C	9.2714311652	14.1087787029	4.5314513885	H	13.5151016393	8.8235017517	13.8556885294
C	7.4884373165	14.5072300586	14.1310636523	H	12.9587758393	5.6895773777	8.9317819088
C	4.6761200121	5.8774937300	9.0057436904	H	7.3364367482	15.7660440482	12.3816210726
C	5.0538740667	9.1809708128	9.7827688970	H	5.8046870705	15.5487309053	13.2653383095
C	12.5597382860	8.4650313811	5.7882499339	H	16.8814946454	12.4074021405	10.0380162820
C	13.7544741001	13.4788291940	12.0012751576	H	17.0460881136	14.0126370809	9.2684688759
C	10.0280509580	6.0582693101	12.9959404319	H	13.2707692775	6.8788202110	14.8795080580
C	3.9125676176	7.1571410854	9.4253821438	H	12.4678830372	7.1032181536	16.4596583180
C	13.2459932443	6.2571732782	5.3433616025	H	14.0322108582	5.1778132122	7.0596083414
C	15.8416098325	14.0259797144	11.0582015802	H	13.0905780804	4.1825851846	5.9115717517
C	11.2612076002	6.0635617122	15.0097612469	C	8.3755614984	9.1359771793	12.2596730940
C	7.0837774827	13.5648560801	11.1086320573	H	7.9490301534	8.3557531116	12.8939317830
C	14.9270936348	11.8737660317	8.5837613753	H	9.4701857818	9.0448827923	12.2817290674
C	12.5484459028	9.1864048605	14.2484552826	H	8.0166798960	8.9885195650	11.2317800764
C	11.9818214521	5.5940772130	8.4261414351	O	7.9269799360	10.3981227643	12.8140396301
C	6.7032331215	15.0339724485	12.9072219234	H	8.2478732494	11.1113678150	12.2351454980

“TS inside” one EtOAc molecule, first rotation from 1-T_d-R

E = -478.9141216882 Ha

H	6.9743398390	10.1702402616	8.2413543465	C	9.0743511294	7.1293356027	5.9261553664
H	6.4026269121	8.6290001354	8.9112121979	H	9.9159710059	6.4357186259	6.1009990587
H	6.5432643988	10.0538702380	9.9635609272	C	9.2058277044	6.0071677645	11.8605739443
C	6.9981264998	9.5221522459	9.1231003150	C	7.3206214505	6.0551513898	10.3104998528
H	8.8789206297	8.5213300078	8.6486173162	N	5.2164691112	11.2473458227	13.3995407601
H	8.5176717414	8.5792664541	10.3836502762	C	4.0392817580	10.4256983358	13.6752928041
C	8.4310766672	9.1238841952	9.4413211151	H	3.4235473540	10.2395509269	12.7781373870
O	9.1991073316	10.3772140673	9.5762121399	H	3.4243493332	10.9556953624	14.4161483339
O	11.1696079989	9.2267193637	9.4034834884	C	6.7041047234	4.8334385775	6.8143242191
C	10.5562688314	10.2783293560	9.5365350253	H	5.7506623482	5.3804256628	6.7109476140
H	12.1843850688	11.6641945793	9.3275059645	H	6.5002141698	3.7590125681	6.7011442097
H	10.5525893819	12.3876260990	9.1187787550	C	8.4534119648	6.7760311870	12.7743421444
H	11.1401643697	11.9541576015	10.7302949366	H	8.9068422316	7.0418197594	12.7253697487
C	11.1536194773	11.6627409274	9.6743130843	C	6.7289447766	5.7306952526	8.9974951964
N	8.0127096417	13.1915965695	5.5976949759	H	5.7242064115	6.1503328903	8.8122031044
N	8.6527066509	14.4776177336	8.0145255329	C	4.4699216220	9.0750167370	14.2916792071
N	10.5803577776	14.8502715288	13.2621751862	H	5.0973207627	9.2643529260	15.1799086176
C	8.7988106149	10.9128622576	5.8024240092	H	3.5642210479	8.5406607401	14.6105257267
C	8.6659697260	13.6098877175	12.4369060190	C	6.3683168708	7.9502884833	13.4588733595
C	6.6800570737	13.0042566516	10.5422150430	H	6.9189432294	8.2541268066	14.3663122876
H	5.9167984901	12.7857822718	9.8002748910	C	10.5564587913	5.5130185917	12.1989636026
C	8.7411037865	14.1289943607	11.1263931929	H	11.1429372021	5.1062174632	11.3575920987
H	9.5765418515	14.7768772301	10.8741158898	C	7.6697185747	5.2529334409	5.6851286659
C	8.4448333677	9.5612487872	5.7900545404	H	8.6081961693	4.6798894434	5.7851236659
H	7.4089073137	9.2583278790	5.6631565032	H	7.2050210834	4.9941591740	4.7236741933
C	7.7502322066	11.9427778661	5.6903822649	N	13.3753179756	10.7704707245	5.3998604861
H	6.7110438998	11.5679860166	5.7090319571	N	15.1474562243	10.7041140036	8.1039724235
C	6.5928718692	12.4693094054	11.8315744684	N	13.5762519801	7.0848454955	13.2378037597
C	7.7493786504	13.8480939120	10.1812174226	C	11.1284431600	10.2929092321	6.1533145143
N	13.1991050519	13.5002807325	13.5768290744	C	13.5634077236	9.3697119710	12.4825898568
C	12.9793813112	14.9196644278	13.8488290238	C	14.3054289550	11.4447974428	10.7580559455
H	13.1738892321	15.5613070215	12.9713123935	H	14.5957533051	12.2367095952	10.0723827398
H	13.6587989156	15.2207891271	14.6586728179	C	14.0738690446	9.0744270173	11.2030368113
C	7.0438038389	15.1456789720	6.7263037845	H	14.1585102494	8.0352721606	10.9003089477
H	8.0250705151	15.6460734436	6.6487033915	C	10.1532795890	11.2707885025	5.9718064477
H	6.2563691227	15.9047077212	6.6203915971	H	10.4178957576	12.3237087427	5.9766673125
C	7.5931899985	12.7777558209	12.7777945531	C	12.5543429109	10.6865978679	6.3733154446
H	7.5059744671	12.3672403391	13.7801326493	H	12.8411289093	10.8534528706	7.4180501676
C	7.8255987909	14.4781865212	8.8464362341	C	13.7697646411	11.7508995245	12.0107241533
H	8.7806063260	14.9847169823	8.6187656566	C	14.4329546384	10.1062252223	10.3305946597
C	11.5288147415	15.1374907802	14.3368950429	N	11.0020999224	5.5185758945	13.3976246266
H	11.3530468735	14.5248182036	15.2387388621	C	12.3454627957	4.9987430017	13.6567912619
H	11.4174823664	16.1967162482	14.6097154489	H	12.8333396804	4.5936234085	12.7531695557
C	9.6784987988	13.9616283724	13.4566855464	H	12.2518943072	4.1910033870	14.3958738691
H	9.5951373793	13.4215998799	14.4166087836	C	15.5259516150	10.3237527418	6.7413913565
C	5.4340207691	11.6297495080	12.1977788286	H	15.3856415300	9.2461819369	6.5418380262
H	4.7502140874	11.3694556897	11.3704452955	H	16.5968692381	10.5487443445	6.6278264493
C	6.8991760030	14.1357185219	5.5660481262	C	13.3914321423	10.6998718150	12.8684282365
H	5.9128464932	13.6426877089	5.6261514110	H	12.9751898935	10.9461745607	13.8414703484
H	6.9508768486	14.6972157943	4.6221529246	C	14.8682409045	9.7898377959	8.9575640568
N	7.8885069751	6.7009176921	5.6992736247	H	14.8956004174	8.7177375347	8.6974241790
N	7.3418885538	5.0387039714	8.1134317222	C	13.2399693213	6.1093434725	14.2600012147
N	5.1406414170	8.2635101487	13.2782904772	H	12.7269829953	6.5515222655	15.1322074220
C	9.4212915250	8.5614029567	5.9549857021	H	14.1735459792	5.6422954892	14.6058690493
C	7.1423732397	7.1639212828	12.4769951892	C	13.2319509300	8.2991961777	13.4342762549
C	8.6421354298	5.6760715341	10.6257453991	H	12.7045245553	8.6147307986	14.3512166777
H	9.2075153745	5.1098645047	9.8907424115	C	13.5750004478	13.1580566973	12.4024552479
C	6.5787164787	6.7878570928	11.2408266907	H	13.7679912788	13.9048033790	11.6118410392
H	5.5622356327	7.1011717335	11.0189201058	C	14.7797577176	11.1567241862	5.6722899432
C	10.7579352090	8.9390562028	6.1512201772	H	14.8194885449	12.2174515432	5.9579659559
H	11.5161883123	8.1767632332	6.3124393963	H	15.3194417877	11.0531573387	4.7240134061

“TS outside” one EtOAc molecule, first rotation from 1-T_d-R

E = -478.9124965847 Ha

H	6.8493233116	10.0538360470	8.3922353256	C	9.0000984913	6.9722759806	5.9427147019
H	6.3569181847	8.5316906924	9.1622516529	H	9.8623761703	6.2965482532	6.0784723448
H	6.6624538926	9.9701550154	10.1562074297	C	9.2586683262	6.0178802472	11.9447726657
C	6.9886445205	9.4172809717	9.2720489849	C	7.3468395729	5.9705538876	10.4311842036
H	8.7563249985	8.3319851287	8.5937411467	N	5.3200145832	11.2495010439	13.5002576057
H	8.6729873704	8.5313551990	10.3517158861	C	4.1235125813	10.4539496384	13.7601324461
C	8.4493879872	9.0094586071	9.3942906401	H	3.5173048047	10.2753733543	12.8549455410
O	9.2337167528	10.2481799142	9.2978024052	H	3.5077953794	10.9965170201	14.4907315690
O	11.1680808855	9.0377150252	9.1246492552	C	6.7115055255	4.6282715244	6.9893189159
C	10.5911890895	10.1158363474	9.1577850838	H	5.7390877015	5.1424200480	6.8953955353
H	12.1100364524	11.4053982775	8.4010579298	H	6.5416702662	3.5460750256	6.8957747545
H	10.5415733387	12.2278919766	8.7204536775	C	8.5083916705	6.8048558319	12.8442699485
H	11.5942810034	11.7535849526	10.0720584777	H	8.9754151018	7.1175595279	13.7747562764
C	11.2494829992	11.4719398919	9.0701862273	C	6.7494378438	5.5959002954	9.1359645697
N	7.9308341150	13.0374434165	5.6107593657	H	5.7373068043	5.9949391284	8.9439623507
N	7.0718571402	14.3815344612	8.1783919360	C	4.5264296726	9.0966985438	14.3803135173
N	10.6100265882	14.8690840822	13.5421910457	H	5.1520348581	9.2758340731	15.2719128916
C	8.6942704617	10.7564171904	5.7726523842	H	3.6111900095	8.5761636177	14.6938144579
C	8.8395346645	13.5147665378	12.5865800309	C	6.4279942547	7.9830260289	13.5269817746
C	6.9052991186	12.8954925830	10.6531406331	H	6.9956474024	8.3167786996	14.4130008656
H	6.1584298645	12.6791676117	9.8947207948	C	10.6141206833	5.5391814445	12.2746125241
C	8.9567238808	14.0213674813	11.2741172560	H	11.2031639144	5.1541433456	11.4242790938
H	9.7970024235	14.6695019168	11.0389347003	C	7.6366587045	5.0595958988	5.8306420213
C	8.3447407858	9.4075716604	5.8898893605	H	8.5958633763	4.5197793108	5.9153664153
H	7.3053434494	9.1111710692	6.0002893592	H	7.1554103004	4.7642100507	4.8875866997
C	7.6571650861	11.8063164379	5.8256858269	N	13.2025637695	10.8676764443	6.3628383184
H	6.6355169482	11.4657730562	6.0697751691	N	15.2178199948	10.8063361854	8.4812425338
C	6.7824381410	12.3728867995	11.9422608476	N	13.5734713451	7.1398783633	13.4597107204
C	7.9919739517	13.7245808738	10.3086457755	C	11.0401890670	10.1248667640	5.6053355428
N	13.2036932758	13.5602672324	14.0357322326	C	13.4742944421	9.4503347719	12.8028081625
C	12.9570919756	14.9698174730	14.3218917444	C	14.1666300328	11.5745236799	11.1106643184
H	13.2199441694	15.6323893002	13.4783978246	H	14.4312749552	12.3881301109	10.4395186361
H	13.5585504270	15.2605051868	15.1943368499	C	13.8607273296	9.2046328015	11.4680187744
C	7.2180282141	15.0309485162	6.8781304190	H	13.8794957555	8.1785681464	11.1130869915
H	8.2280983153	15.4444415743	6.7107014951	C	10.0508294391	11.1044229598	5.6019290661
H	6.4931106630	15.8559790856	6.8338240202	H	10.3102813876	12.1530924068	5.4961612893
C	7.7662558653	12.6773037989	12.9048258047	C	12.4708619922	10.4991610503	5.3907317167
H	7.6571074911	12.2732800544	13.9074276219	H	12.8389326706	10.4801918201	4.3467028562
C	8.0794777276	14.3316093698	8.9652511457	C	13.7326992712	11.8419852805	12.4132310379
H	9.0528496789	14.7821304956	8.7010059637	C	14.2214567925	10.2542564933	10.6208412743
C	11.4666407433	15.1682831195	14.6888124724	N	11.0629303029	5.5253162401	13.4718015032
H	11.2264322756	14.5460290022	15.5689116835	C	12.4074882029	4.9995191259	13.7041190465
H	11.3192440916	16.2237572196	14.9577659754	H	12.9055113131	4.6657053100	12.7775968719
C	9.7779344620	13.9038288407	13.6559044977	H	12.3155411908	4.1360537413	14.3794436950
H	9.6894428103	13.3269069807	14.5935620081	C	15.5006685515	10.4111023456	7.1020931699
C	5.5973542439	11.5682163361	12.2926666060	H	15.3472059534	9.3300398554	6.9300292965
H	4.9410434809	11.2856392637	11.4511889300	H	16.5491349777	10.6497896141	6.8784451307
C	6.8772388474	14.0391796248	5.7378371069	C	13.3865138057	10.7672250306	13.2588697276
H	5.8814629365	13.6004717387	5.9267388885	H	13.0534406934	10.9854118638	14.2698439972
H	6.8370800391	14.6064223532	4.7973376060	C	14.6205947499	9.9574226379	9.2313456696
N	7.8117982045	6.5148681058	5.8039295980	H	14.3583773450	8.9478388090	8.8758208104
N	7.3634353198	4.8763038055	8.2741961462	C	13.2785538553	6.0658319666	14.4010427568
N	5.1917342497	8.2742434773	13.3703188232	H	12.7667307982	6.4145712905	15.3152004000
C	9.3332716474	8.4057811617	5.8766533704	H	14.2298747440	5.5972972567	14.6915584004
C	7.1868632528	7.1652810235	12.5560395775	C	13.1980322401	8.3323858622	13.7256483196
C	8.6767264137	5.6214943398	10.7391515045	H	12.6836211065	8.5913681149	14.6678357266
H	9.2399640344	5.0383606499	10.0161527741	C	13.5709037164	13.2403098664	12.8518375902
C	6.6080391108	6.7268414590	11.3463543884	H	13.7573827009	14.0057525705	12.0771359664
H	5.5829541865	7.0150871024	11.1295500517	C	14.6040208594	11.2081657233	6.1247238083
C	10.6809586778	8.7771190000	5.7585703405	H	14.7302828646	12.2784920081	6.3346279355
H	11.4550803874	8.0137585844	5.7817242338	H	14.9257763002	11.0141606873	5.0843800766

“TS inside” one CCl4 molecule, first rotation from 1-T_d-R

E = -484.8272653461 Ha

N	7.4411320752	13.3095205617	5.9786477164	C	16.3702097693	13.1746237191	9.7605105782
N	10.1487095715	12.8486163820	4.9410805932	C	12.1381403882	7.1874781879	15.4165707275
N	8.9315989395	14.1571472775	13.6629076360	C	13.1276129834	5.0561241509	6.5078722211
N	5.9527795228	5.8893135477	9.5653913935	H	7.6428595504	12.6269391427	3.9536357590
N	4.4132397767	8.2995265939	8.8228234534	H	7.1949293487	14.3429831137	4.1852454742
N	15.2387901206	12.9262811117	8.8683912148	H	5.6677686317	9.9698550004	7.2288131058
N	15.0155304903	13.0954288631	11.8116250808	H	10.9018175156	10.4174085360	5.3016390580
N	10.9773497736	6.0834594511	13.5478323568	H	11.3088318559	14.2422579556	12.7339473966
N	6.3982834607	14.2065092943	11.6389324980	H	7.6173836078	6.4655352820	11.4940624729
N	13.4133511821	7.4467367869	5.9746359908	H	9.4370713026	14.8693238341	5.0840491466
N	11.7618754702	8.5545932254	15.0610039384	H	9.5277035090	14.1563619376	3.4466290469
N	11.8924759827	5.2377715083	7.2635085068	H	5.8572642482	10.9071911414	11.4202381722
C	6.6266023406	11.8483584814	7.7247409973	H	14.3919081048	9.2699101129	7.5408887212
C	11.8314920319	11.9900797048	6.4374123594	H	14.0671577891	10.9316128714	12.8345873458
C	10.6666316591	12.5068299201	13.8410573719	H	11.8917527131	6.1417758809	11.1189352006
C	8.3544847716	6.1390495489	9.4979042457	H	6.9337818011	13.8019607596	14.3691511895
C	5.9636491049	10.6535368764	8.0204914853	H	7.6108847379	15.4249278105	14.6503475357
C	11.7136182854	10.6648102348	5.9802093511	H	7.5178639836	13.6325564441	8.5335017610
C	11.5758551574	13.2403067302	13.0561342836	H	12.9782271955	13.3311462171	7.6854305643
C	8.5078850523	6.3345439726	10.8852621228	H	10.2773515183	10.6327326044	14.8439937505
C	5.6668697309	10.3110945981	9.3524799273	H	9.3975794674	5.8117901698	7.6308109362
C	12.6323674867	9.6917072242	6.3747734788	H	4.7871036184	5.8631328033	7.7620676623
C	12.8161187774	12.6789899148	12.7276052119	H	6.7909158054	11.3681163088	5.5919186334
C	9.7768646704	6.3248543845	11.4688297178	H	10.9436064733	13.9984725214	6.4902658341
C	6.0668474886	11.1721190895	10.3861648169	H	8.7069145122	12.4256364578	14.8068857385
C	13.6826377275	10.0402299027	7.2487217181	H	6.9956328401	6.1313244011	7.7769908138
C	13.1104466234	11.3565629084	13.1261091708	H	4.1489342760	4.9326043366	9.1497710119
C	10.9109460846	6.1491738077	10.6519710195	H	4.9038953127	8.8340148389	10.7727362618
C	6.7191191507	12.3804658062	10.1008441751	H	11.5756082347	8.1297903906	5.2639815880
C	13.8145676552	11.3504439208	7.7135180616	H	13.4343795272	14.4302360405	11.5658803680
C	12.2017170892	10.6134886461	13.8832313941	H	9.0119655138	6.7787793713	13.4751979329
C	10.7761211777	5.9569935060	9.2762235282	H	3.6753921870	7.0328506344	10.3920007975
C	6.9978444219	12.7112533599	8.7757074057	H	2.8144883010	6.9566934454	8.8259083131
C	12.8700488872	12.3157758916	7.3144068520	H	12.2934495501	6.0653669382	4.7688228501
C	10.9818085341	11.2113237503	14.2528463099	H	14.0728072942	5.8936241163	4.7579589482
C	9.4891500083	5.9663456606	8.7025354025	H	15.4232287852	14.8901100228	10.7089365479
C	6.9661864462	12.1743419025	6.3270314437	H	16.7850742956	14.1780467738	11.6218912677
C	10.9080600514	13.0340054916	5.9541558018	H	10.0616032553	6.5392251494	15.4372565152
C	9.3499332361	13.0550528390	14.1659555248	H	11.2662771264	5.2163068826	15.4151868765
C	7.0184708513	6.0615791045	8.8789608500	H	8.2174307417	13.1728457761	11.5201071572
C	7.8072482033	13.5204939379	4.5818322402	H	15.5428496736	10.8660493065	8.9704626236
C	9.2899852502	13.9444650120	4.4985949203	H	13.4670452724	8.8183405494	13.8878023486
C	7.5610808429	14.5968101604	13.9267443161	H	12.9434866721	5.8987287599	8.9393666513
C	4.6726503373	5.8536594293	8.8598511016	H	7.5768059514	15.8720033672	12.1781328140
C	4.9521550178	9.0678099574	9.6942111926	H	6.0068263026	15.7431903429	12.9762684539
C	12.4999644206	8.3327539345	5.8330193907	H	16.8793961472	12.2457827286	10.0729363784
C	13.8033072820	13.4728538794	11.9743481927	H	17.0949995455	13.8063895145	9.2281202714
C	9.9086111478	6.4276369101	12.9338009924	H	13.0922069017	6.8687494885	14.9613175954
C	3.8018000084	7.0597327278	9.2953867892	H	12.2407636311	7.1429431204	16.5100293635
C	13.2043445633	6.1251265861	5.3900132517	H	14.0331741907	5.1268555813	7.1356424662
C	15.8994289988	13.9424587721	11.0160540173	H	13.1044361783	4.0646400423	6.0363704664
C	11.0189197697	6.2039738411	15.0007315292	Cl	9.3636098911	9.6430133741	8.6284354716
C	7.1771412194	13.3001781591	11.1902641222	C	10.2279652187	10.2963117152	10.0622385885
C	14.9457097431	11.7124942038	8.5862937045	Cl	11.8521277135	9.5253973243	10.2081206520
C	12.5246234249	9.2310609362	14.2888240930	Cl	10.4335490026	12.0831011570	9.8905781294
C	11.9719331684	5.6966698580	8.4554820845	Cl	9.2621085678	9.9435961764	11.5517416576
C	6.8826092216	15.1668260965	12.6568062243				

“TS outside” one CCl4 molecule, first rotation from 1-T_d-R

E = -484.8286869683 Ha

N	7.1664941729	13.5502055876	5.8804523336	C	16.3454566014	13.2211908798	9.5844335866
N	9.9597444104	12.9007708822	4.9337384847	C	12.1294829180	7.2209402786	15.3713227588
N	8.9419189771	14.1265197580	13.7818982247	C	13.1971970187	5.1606838003	6.4449281090
N	5.9888886176	6.0890304078	9.5144368795	H	7.5024659668	12.7242575988	3.9244504412
N	4.3960171089	8.5436842560	8.8360344009	H	7.0861755443	14.4601735113	4.0099017029
N	15.2217321811	12.9865372586	8.6772940277	H	5.8093512334	10.1120742536	7.3358794990
N	14.9674471189	13.0444409104	11.6219436638	H	10.8049531542	10.4421787710	5.2115532332
N	10.9878420791	6.0543322953	13.5483096474	H	11.2129628266	14.0988507866	12.3978508914
N	7.0153680788	14.2326958537	11.6337911066	H	7.6715580215	6.4773026047	11.4631559154
N	13.4292682341	7.5277228306	5.7979203340	H	9.2965543928	14.9390274558	5.0992481540
N	11.7286014755	8.5557746515	14.9538657844	H	9.4268499431	14.2561346460	3.4536268272
N	11.9674890057	5.3330045826	7.2127719014	H	5.0678631321	11.5444698924	11.3154272395
C	6.3203398135	12.1836118141	7.6878366700	H	14.3321293121	9.3323563567	7.4171928231
C	11.7303896641	12.0282771519	6.3356252899	H	14.0544811431	10.8806771319	12.7236221930
C	10.5083768012	12.3348132359	13.4103013602	H	11.9454708043	6.1338807386	11.0992060892
C	8.4088617346	6.1586919532	9.4671440456	H	6.8820850860	13.7636571313	14.2820429451
C	5.8329462860	10.9262226813	8.0548590306	H	7.5671121352	15.3338545318	14.7918908613
C	11.6227545051	10.6983393062	5.8796537470	H	6.7099029677	14.1979395153	8.3459615536
C	11.4770123179	13.0981682552	12.7286944044	H	12.8986321871	13.3904546104	7.5429266236
C	8.5617002917	6.3355879002	10.8565093978	H	10.0980202701	10.4346117639	14.3533365396
C	5.3478999830	10.6927087510	9.3514170834	H	9.4563492389	5.8410265066	7.6000426361
C	12.5632520827	9.7351737637	6.2548771599	H	4.8471500607	6.1848654103	7.7008446945
C	12.7502740163	12.5753631030	12.4774391471	H	6.8316221450	11.5034919846	5.6698683821
C	9.8279737315	6.3120711131	11.4450361002	H	10.9085476217	14.0590218995	6.3839830496
C	5.4026100348	11.7260502550	10.2959736811	H	8.3731400269	12.1203860536	13.8659488602
C	13.6114658492	10.0930489657	7.1291178287	H	7.0681371501	6.1939882388	7.7353030651
C	13.0610985539	11.2744828440	12.9222034370	H	4.1937858182	5.1706019938	9.0160960226
C	10.9653316198	6.1434192825	10.6297212163	H	4.6304265293	9.2074720338	10.7991035685
C	5.8714984084	12.9983980423	9.9346092151	H	11.5216230578	8.1207726054	5.1936852565
C	13.7411325442	11.4107300589	7.5801702140	H	13.3724247509	14.3612158342	11.3774009731
C	12.1143221949	10.5144729850	13.6115441689	H	9.0418875136	6.7920248312	13.4356704720
C	10.8336815087	5.9664783662	9.2494386139	H	3.7215485532	7.2128469129	10.3814070579
C	6.3253116129	13.2253705974	8.6374096088	H	2.8429675885	7.1591655780	8.8239615869
C	12.7877419252	12.3708900477	7.1834009051	H	12.3027213977	6.0744153500	4.6833865017
C	10.8297546475	11.0459403363	13.8331527428	H	14.0845459884	5.9290113635	4.6304491321
C	9.5460338404	5.9787993367	8.6742058781	H	15.3662937593	14.8847347577	10.5903282541
C	6.8068189493	12.4006981935	6.3135055940	H	16.7283631444	14.1570373180	11.4901607938
C	10.7997191786	13.0815082730	5.8813350729	H	10.0581148232	6.5412557677	15.4251457719
C	9.1665877251	12.8704445062	13.7037458507	H	11.2808059092	5.2324058621	15.4401264436
C	7.0743722091	6.1531391362	8.8391682430	H	5.0374445363	14.6848428148	11.1386746888
C	7.6454696739	13.6538442459	4.5032703853	H	15.4408635570	10.9242290688	8.8735119593
C	9.1419935431	14.0299590370	4.4917325360	H	13.4094461397	8.7483108320	13.7338748341
C	7.5698044570	14.5800043650	13.9934407751	H	13.0044618810	5.9238825522	8.9256989215
C	4.7213689865	6.1102587615	8.7956671596	H	7.7801818685	16.0123429976	12.3954327277
C	4.7641910552	9.3932669005	9.7183691008	H	6.0803469580	15.7240056478	12.8742803624
C	12.4679967565	8.3683987930	5.7063744702	H	16.8690697218	12.2906611860	9.8651721706
C	13.7465299288	13.3993173460	11.7705087535	H	17.0600942707	13.8861519381	9.0805071595
C	9.9392203124	6.4163093301	12.9128522781	H	13.0850270412	6.8917857483	14.9269433955
C	3.8343400299	7.2732571886	9.2844518358	H	12.2360518944	7.2228078253	16.4656916576
C	13.2298713820	6.1755827952	5.2740481694	H	14.1099379760	5.2814636627	7.0542442265
C	15.8516013384	13.9323602822	10.8677755328	H	13.1913758900	4.1488723736	6.0173601835
C	11.0192434642	6.2041549387	14.9999287044	Cl	9.1061865289	9.6177770888	8.2325090479
C	5.9458290377	14.0758061047	10.9657319143	C	9.6655602337	10.4094565875	9.7611195982
C	14.8787686207	11.7745287076	8.4478189405	Cl	11.3661469702	9.9173202765	10.0969351778
C	12.4652523138	9.1775645170	14.1136086958	Cl	9.5642028258	12.1943747527	9.5990376954
C	12.0372697220	5.7406513874	8.4257087459	Cl	8.5998368878	9.8762220562	11.1284563127
C	7.0580720273	15.2409367946	12.6931791981				

“TS outside” gas phase, second rotation from 1-T_d-R

E = -456.157459051863 Ha

N	7.2600267367	13.4322783316	6.0595070360	C	12.3822043623	9.5969967566	14.0522846104
N	9.9987669551	13.0878243763	4.9574597247	C	11.9449384432	5.9254751678	8.2412088168
N	8.5056115599	13.4613862772	13.4812020231	C	6.9367922826	15.0474896493	12.4377542030
N	5.8725024094	5.7034065762	9.0077486936	C	16.5081189833	13.2091412874	9.4328193656
N	4.3076178999	8.0975478977	8.3133739889	C	11.8202978539	7.6261111234	15.2266945961
N	15.3306286075	13.0124127740	8.5854970771	C	13.1881177695	5.2818516309	6.3341642322
N	15.2007348338	13.2594710314	11.5221869902	H	7.4908558299	12.9174356526	3.9866503622
N	10.7012389365	6.6037033843	13.2729631864	H	7.0181898793	14.6019464156	4.3546930777
N	6.7038496103	14.2773515297	11.2087772390	H	5.6071903286	9.9242067139	6.9545222155
N	13.4137646922	7.6363224313	5.6895203453	H	10.7871037040	10.5917550236	5.1869317373
N	11.5938443994	9.0244847750	14.8804863229	H	11.6518368366	14.6785562704	12.4787720250
N	11.9311605764	5.4214022295	7.0645164956	H	7.4009005737	6.3782365010	11.0658902932
C	6.3954603902	11.8215223442	7.6500122916	H	9.2576061471	15.0734930952	5.3105535415
C	11.7497720042	12.1398042833	6.3358695615	H	9.3393782177	14.5301385457	3.6101754253
C	10.8605438775	13.0360026236	13.6509009707	H	5.4319896043	10.5514385319	11.1988904842
C	8.2648269098	6.0660179465	9.1160595862	H	14.3871381989	9.4179518127	7.2327847220
C	5.7936292711	10.5655096015	7.8124039453	H	14.0362787347	11.1011775610	12.5062182438
C	11.6248556492	10.8235583795	5.8398843035	H	11.7053247201	6.4452429170	10.9017249623
C	11.8117681764	13.6566050457	12.8161602210	H	6.5112868813	13.6356546572	14.0606456891
C	8.3295203741	6.3055458679	10.5054389268	H	7.4907692262	15.0430820058	14.5356080731
C	5.4235680331	10.1044774445	9.0888536571	H	7.0593729327	13.6166169084	8.6523141014
C	12.5743686282	9.8478880511	6.1583059040	H	12.9491175983	13.4612637427	7.5610169335
C	12.9631617969	12.9628831712	12.4077447328	H	10.3187690093	11.2273096934	14.6806100156
C	9.5650027415	6.4387609238	11.1481695122	H	9.4263131402	5.7910248875	7.3128841181
C	5.6888821306	10.9123533402	10.2035832364	H	4.8566451534	5.7394579191	7.1165715644
C	13.6546552312	10.1858743122	6.9996069231	H	6.6673540754	11.5148185985	5.4974623345
C	13.1403304247	11.6291733384	12.8240251158	H	10.8583171044	14.1325555039	6.5431246180
C	10.7522828174	6.3421437135	10.3903560953	H	9.7135693033	14.6331069865	14.7124797480
C	6.2534972465	12.1932529729	10.0553557417	H	7.0392575778	5.9916121178	7.3073427217
C	13.7959645450	11.4817764991	7.4997382861	H	4.1471979077	4.7023278215	8.3899996773
C	12.1914821093	11.0003273334	13.6382903482	H	4.6605016508	8.4730383576	10.3312118226
C	10.7014712449	6.0958307037	9.0168496178	H	11.5177276837	8.2555313124	5.0720263704
C	6.6068113323	12.6389877986	8.7758757220	H	13.6623564920	14.6109010472	11.1428364639
C	12.8273342914	12.4544404605	7.1705213109	H	8.6343919233	6.8305251397	13.0951255926
C	11.0547739923	11.7222826885	14.0554606949	H	3.4929132540	6.6895044541	9.7146378749
C	9.4489396196	5.9741687754	8.3836410187	H	2.7686694571	6.7056799333	8.0789848003
C	6.7974965075	12.2640777841	6.2993378295	H	12.3059477347	6.1821221109	4.5538556780
C	10.8018891904	13.2050671554	5.9463928184	H	14.0902591413	6.0472370946	4.5260701675
C	9.6192130582	13.7833056353	14.0163803354	H	15.6999202660	14.9980020981	10.3656826003
C	6.9819514866	5.9123847572	8.4072679471	H	17.0352099988	14.2244898225	11.2661234413
C	7.6407122658	13.7586919388	4.6865556445	H	9.6926859469	7.1824541831	15.0782367568
C	9.1164409058	14.2096885056	4.6378912016	H	10.7607752114	5.7568753728	15.1650585785
C	7.3281886055	14.2948257159	13.7375854698	H	6.4306126618	12.4557155427	12.2036247114
C	4.6557623968	5.6571983176	8.1990236162	H	15.5459112411	10.9435009732	8.6969007155
C	4.7608922767	8.8025102744	9.2817819296	H	13.2502071020	9.0746945034	13.6133467191
C	12.4626638167	8.4873130853	5.5938392481	H	12.8817930267	6.2191247606	8.7450450633
C	13.9923977984	13.6713828036	11.6208858629	H	7.7375150000	15.7632508352	12.2061028063
C	9.6093246832	6.6481905287	12.6082345543	H	6.0360387906	15.6515089230	12.6267795108
C	3.7087040833	6.8023515139	8.6378552007	H	16.9740021602	12.2580090743	9.7443204789
C	13.2244557816	6.2902449817	5.1563190807	H	17.2466961691	13.7907393560	8.8638577967
C	16.1223364005	14.0299169992	10.6872475307	H	12.7638392049	7.2241268516	14.8161978301
C	10.6481380642	6.7589277574	14.7232610398	H	11.8571592360	7.5507401631	16.3223748005
C	6.4742986879	13.0196429940	11.2613248556	H	14.0786372334	5.4396796269	6.9669043514
C	14.9710742518	11.8113919360	8.32744498781	H	13.2271280321	4.2662550600	5.9187484536

“TS inside” gas phase, second rotation from 1-T_d-R

E = -456.156026627552 Ha

N	7.0915305613	13.2731483467	6.1672217199	C	12.2871491921	9.5614809270	13.6452948382
N	9.9255931431	12.9961734229	5.1222243622	C	11.8268790260	5.7728450972	8.0293805543
N	8.7422903307	13.8911779069	13.5822854379	C	6.8056487521	15.0516746725	12.2794435415
N	5.7644959595	5.6017138847	8.9656508349	C	16.6731873110	13.1923600692	9.2264159908
N	4.1214428760	7.9233087817	8.3416274136	C	11.7084226916	7.6896693222	14.9566936648
N	15.5026355828	12.9902310668	8.3726502910	C	13.0948168494	5.1757499338	6.1369736951
N	15.2792479216	13.1844425168	11.2561239120	H	7.4695351017	12.7658757053	4.1134528864
N	10.6600779265	6.4361636042	13.1054389952	H	6.9210187902	14.4330686476	4.4523813665
N	6.5303993461	14.1600638541	11.1451574415	H	5.4731298480	9.7355674291	7.0359917199
N	13.4476838714	7.5598832739	5.6104593260	H	10.8218404638	10.5343503915	5.1951059852
N	11.4132865216	9.0059094289	14.3959041780	H	11.5422223411	14.4557549165	11.5845073057
N	11.8148037464	5.3283364101	6.8281516857	H	7.3472189641	6.3258759967	10.9383072155
C	6.2070953703	11.6543893170	7.7333828769	H	9.1050536504	14.9294063745	5.5834239193
C	11.8140030882	12.0800812899	6.3214785053	H	9.2541966125	14.4981925233	3.8568898122
C	10.5982986132	12.7607718328	12.5312404917	H	4.9895241133	10.4763289127	11.2408070521
C	8.1582837920	5.9722595702	8.9753634252	H	14.5274857366	9.3872021357	7.0623265619
C	5.6006480799	10.3998053054	7.8869615135	H	14.1346895069	11.1307632904	12.4222743454
C	11.6898558283	10.7719502580	5.8046943596	H	11.6461414530	6.3256112719	10.6750753556
C	11.6875765316	13.4528903242	11.9812545381	H	6.7257716003	13.7018282514	14.0206518799
C	8.2615558290	6.2385737108	10.3569440579	H	7.3995774561	15.2854882531	14.3260345332
C	5.1411372659	9.9718591691	9.1459536436	H	6.8149776270	13.4630978402	8.7358816789
C	12.6626467896	9.8024996829	6.0713515209	H	13.0597132616	13.4101348158	7.4889225768
C	12.9631912739	12.8704998145	11.9431806799	H	9.9577902103	10.9185477225	13.4605092183
C	9.5123673679	6.3606585954	10.9712978836	H	9.2708871090	5.6552097675	7.1467951411
C	5.3217091147	10.8111757177	10.2586456589	H	4.6768235825	5.5648278142	7.1144818804
C	13.7771170302	10.1481219306	6.8645541197	H	6.6574747181	11.3106970438	5.6117421462
C	13.1434655325	11.5753179462	12.4619430069	H	10.9019821109	14.0502721700	6.6325320038
C	10.6792075448	6.2342898394	10.1870426500	H	8.7068953074	13.3371992085	11.5606225446
C	5.9120959228	12.0814342330	10.1203184668	H	6.8667267771	5.8286622720	7.2138083367
C	13.9336614578	11.4474123487	7.3544889737	H	4.0515182033	4.5304449386	8.4321929212
C	12.0685564062	10.8837115762	13.0306577445	H	4.3167462678	8.3540770396	10.3686644857
C	10.5936329325	5.9720910461	8.8154074081	H	11.5877152944	8.2455677433	4.9630825899
C	6.3485825924	12.4913678399	8.8518913441	H	13.7856664870	14.5682339365	10.8266789113
C	12.9343384965	12.4067389867	7.0902339410	H	8.6339361807	6.8833213702	12.9098259226
C	10.7889593514	11.4780943142	13.0418122995	H	3.3251329055	6.4931155842	9.7281330755
C	9.3233707522	5.8601979297	8.2127975561	H	2.6099079455	6.5034828797	8.0886615050
C	6.6861506003	12.0829915166	6.4011539037	H	12.3156922595	6.2051649213	4.3864725900
C	10.8115538658	13.1261667888	6.0337989972	H	14.0907348666	5.9924608621	4.4041011909
C	9.2379692470	13.3796173972	12.5239280879	H	15.8541954041	14.9580916555	10.1960075054
C	6.8499768841	5.7936868522	8.3175452394	H	17.1413820751	14.1283844851	11.1194870290
C	7.5489916617	13.6099062307	4.8215179305	H	9.6285096086	7.0513815192	14.8873417028
C	9.0107959125	14.1054037473	4.8551108006	H	10.8208572271	5.7310478931	15.0586820836
C	7.3849280285	14.4684751423	13.5907872579	H	5.9132985720	12.5021615896	12.2800943791
C	4.5182091385	5.4989155595	8.2050453546	H	15.7231822629	10.9238142963	8.4997895098
C	4.4839879677	8.6631200317	9.3212923105	H	13.2630131570	9.0877573581	13.4372519764
C	12.5289901696	8.4461908961	5.5042083442	H	12.7699312619	6.0021444826	8.5552009610
C	14.0735918244	13.6106827523	11.2970226985	H	7.4980529433	15.8185758603	11.9076346608
C	9.5849658811	6.5909897203	12.4295389307	H	5.8715089667	15.5823726501	12.5235173389
C	3.5453292937	6.6161382523	8.6532041405	H	17.1542167991	12.2433843621	9.5214291420
C	13.2179560527	6.2430985210	5.0215663031	H	17.4056553561	13.8018084561	8.6797110729
C	16.2503909715	13.9722738910	10.4971592562	H	12.6956305972	7.3021104133	14.6488637241
C	10.6123969037	6.6826249875	14.5485986619	H	11.6956184393	7.7773710603	16.0524773350
C	6.1104305876	12.9623665121	11.2959928954	H	13.9629954877	5.2597997866	6.8132403425
C	15.1398826266	11.7869786206	8.1328934347	H	13.1114421107	4.1842168066	5.6658599773

“TS outside” gas phase, last rotation to 1-C₃

E = -419.404363575052 Ha

N	7.0852421314	6.6149452954	6.6889539675	H	16.4240322377	10.8466220614	7.4219397303
N	11.3146450117	6.7624638252	14.3108165594	C	14.2320861505	13.5910943680	13.9167417300
N	12.2540360632	5.4278792224	11.6418270044	H	14.9676415604	12.8611192541	13.5359123733
N	9.7886771173	5.5764431479	6.9852057263	H	14.5778636391	13.9515125041	14.8964572133
C	10.2440851619	8.9295118753	14.2174950399	C	10.6482527020	14.3526819569	9.7213736155
C	11.4558788966	9.6490607058	14.1346656786	H	9.9999924347	14.7813842444	10.4845605996
H	12.3904265703	9.0944599545	14.1370121353	C	10.9904356680	13.5639166390	7.4534461476
C	10.6047364457	6.5398567591	6.7848487974	H	10.5873252812	13.3824178955	6.4604888459
H	10.6793375278	7.0380644553	5.8017391906	C	10.1450428914	14.1266460435	8.4288119572
C	11.4912572890	7.0823281127	7.8314887864	C	12.0035106314	14.1124269675	10.0093359285
C	11.3886325804	6.6671846609	9.1690448207	C	15.2472902354	11.8271448942	5.8825498835
H	10.6881274632	5.8816596672	9.4323102521	H	16.0826185880	12.4671335262	5.5678638726
C	10.2406025621	7.4510796147	14.1899482398	H	14.6604621399	11.5482406710	4.9898676233
H	9.2651745261	6.9794095746	13.9757192897	C	14.3940188704	9.4972221631	8.0667936980
C	12.2008632467	6.7104145041	11.5803433258	H	14.9031272355	10.0378236039	8.8833113914
H	12.3475010209	7.3967912166	12.4165271323	C	14.1669311149	14.8145846907	12.9638959653
C	7.4443202813	5.2346823906	6.3637871445	H	13.4611998776	15.5478983285	13.3900993631
H	6.7956814125	4.8931291780	5.5461703085	H	15.1629258423	15.2721486600	12.9281510598
H	7.3324563885	4.5443028599	7.2164060076	N	8.3661209693	14.6832541976	6.8898115203
C	11.2861155472	5.3219860699	14.0495740541	N	6.6170334736	11.2604338021	14.2890500304
H	10.3043813324	4.9771794096	13.6803274766	N	4.8708469783	11.2311722170	11.8465611279
H	11.4977227957	4.7994187150	14.9939729034	N	5.9602908864	12.9521626393	7.0768569369
C	13.0910042503	8.2686276431	9.8134387235	C	9.0232957338	11.0437868531	14.1112660051
H	13.7160162225	8.7292526492	10.5774107595	C	9.0360551547	9.6359618323	14.2060432768
C	12.4543245878	8.0347574448	7.4853465749	H	8.0853931072	9.1102666266	14.2416035695
H	12.5902282737	8.3361510460	6.4504357020	C	6.4379240188	11.7880654344	6.8512511507
C	13.2865243218	8.6073921593	8.4630938062	H	6.9467710104	11.5408470518	5.9026613423
C	12.1696768470	7.2669435791	10.1774110355	C	6.3413996530	10.6864520794	7.8307261722
C	8.9151406590	5.1737271878	5.8859898125	C	5.8811346815	10.9175394868	9.1378217824
H	9.1422221634	4.1306693258	5.6239782188	H	5.5903167287	11.9192984632	9.435239007
H	9.0444964106	5.7974964023	4.9842937840	C	7.7515777509	11.7931612619	14.0354516676
C	6.9016445834	6.9291927946	7.9162861358	H	7.8433812247	12.8509505094	13.7301050840
H	6.9502448262	6.1765055657	8.7225977001	C	5.2752745939	10.0893350023	11.4284181639
C	12.4070700940	4.9072140143	13.0535151701	H	5.2472961073	9.1942399446	12.0754097394
H	13.3760909745	5.2329181814	13.4563231212	C	6.9944594726	15.1395540928	6.6678730594
H	12.4203805463	3.8133380913	12.9944352864	H	7.0234823399	15.9626488833	5.9416720851
N	14.7664181406	9.6097866778	6.8454589943	H	6.5087900509	15.4999653286	7.5913276294
N	12.9004065227	13.0085068816	14.0970785746	C	5.4109776921	12.0720361167	14.1213583261
N	13.7921926657	14.4015061948	11.6081245801	H	5.6208752060	13.0708047207	13.7006192215
N	14.4674815780	12.5474878061	6.8843095562	H	4.9494880470	12.2019409317	15.1110689610
C	11.4653797989	11.0453522144	14.0460295800	C	6.1560078132	8.5664637461	9.6529186885
C	10.2370485407	11.7364848346	14.0300665854	H	6.0806359939	7.7432187869	10.3624567842
H	10.2502010971	12.8193393232	13.9388644240	C	6.7006297075	9.3879588463	7.4441699256
C	13.2022626400	12.6529290590	6.7237198774	H	7.0482436287	9.1865744232	6.4343932560
H	12.6930291650	12.2756564014	5.8193697923	C	6.5962732988	8.3109880449	8.3435482232
C	12.3306369000	13.2706520200	7.7463679565	C	5.7862369640	9.8653996834	10.0580536157
C	12.8329996762	13.5649560815	9.0229527211	C	6.1457052207	13.9932946872	6.0692101979
H	13.8765103583	13.3731742125	9.2470753302	H	5.1588757712	14.4010893780	5.8106634897
C	12.7619289028	11.7472721989	13.9348242150	H	6.6265589017	13.6233685974	5.1464424731
H	13.6242952797	11.0981576119	13.6982465477	C	8.7744863184	14.5629048291	8.0970822805
C	12.5471419718	14.4975212219	11.3193983317	H	8.1324195425	14.8239047996	8.9569229576
H	11.8174243384	14.9090038250	12.0375848834	C	4.3913073974	11.3271739230	13.2260661068
C	15.8421364910	10.5493553463	6.5328196773	H	4.1881929198	10.3396722609	13.6764101961
H	16.5179466229	10.0740286016	5.8110150582	H	3.4579391002	11.9057941479	13.2202850081

“TS inside” gas phase, last rotation to 1-C₃

E = -419.396375705772 Ha

N	7.0016474230	6.5482560471	6.6418348884	C	9.1221731066	11.2160863214	13.9240596011
N	11.1704164609	6.9093282496	14.4751080816	C	9.1415719150	9.8102685690	13.8738319539
N	12.3627499845	5.9108036103	12.1219957470	H	8.1958273371	9.2770127051	13.8378625532
N	9.7549178731	5.2659981179	6.6513809212	C	6.5131797770	11.7834146239	6.8134202887
C	10.3499722729	9.1117489784	13.8947660072	H	7.0610452807	11.5489887471	5.8829509705
C	11.5735020344	9.8152627083	13.8900936546	C	6.4070660044	10.6760231296	7.7885183971
H	12.5040450869	9.2550136798	13.8666664522	C	5.9789507989	10.9067793711	9.1076025722
C	10.3721276508	6.3882866256	6.6667127738	H	5.7171467061	11.9121578422	9.4190520555
H	10.1716358703	7.1851752981	5.9303117229	C	7.8362330813	11.9407469794	13.9217118660
C	11.4534981355	6.6645463838	7.6495866437	H	7.8893354953	13.0241375224	13.7101648740
C	11.6272906312	5.8616981271	8.8005044383	C	5.3958676503	10.0600650984	11.4010412241
H	10.9522472636	5.0236140521	8.9521570087	H	5.4065251942	9.1686771180	12.0534929440
C	10.3069240582	7.6395082732	13.8822644447	C	6.9835953408	15.1719452295	6.6122645611
H	9.4677689240	7.1980436760	13.3143727145	H	7.0028468383	15.9726773031	5.8607803297
C	12.6826293190	5.3695010041	11.0166707072	H	6.4576909516	15.5418434218	7.5095844277
H	12.8978015897	4.2887477393	10.9175793729	C	5.4783810419	12.0930779436	14.0427559090
C	7.3009489181	5.1501700189	6.3410309544	H	5.6105397628	13.1034292881	13.6182789570
H	6.5527845278	4.7895459393	5.6225633231	H	5.0566994999	12.1955995161	15.0533345898
H	7.2746316460	4.4997992832	7.2335956451	C	6.2346988834	8.5516252597	9.6053088856
C	11.1009083715	5.4745450964	14.2087958869	H	6.1726622314	7.7264366350	10.3142011234
H	10.1651759675	5.1801803442	13.6987655807	C	6.7205342782	9.3697159491	7.3819976444
H	11.1681143379	4.9201858913	15.1541922343	H	7.0321379140	9.1676086194	6.3604439355
C	13.4702434865	7.2525026659	9.5241462801	C	6.6235950003	8.2927680373	8.2822007626
H	14.2293551720	7.4944143615	10.2647409201	C	5.8882435316	9.8498540310	10.0240096461
C	12.3454167602	7.7223296042	7.4269103926	C	6.2028117286	13.9811813122	6.0175850300
H	12.2691771495	8.3318719252	6.5300620367	H	5.2125787664	14.3466838232	5.7113935992
C	13.3802092541	7.9996549494	8.3402832554	H	6.7307221547	13.6167320673	5.1184448073
C	12.6118815420	6.1657845202	9.7492789155	C	8.7162548625	14.6711980378	8.1106474544
C	8.6948015256	5.0485522033	5.6682686905	H	8.0399718435	14.9503743518	8.9381866018
H	8.8101461405	4.0323957318	5.2703545154	C	4.4741061592	11.2855489556	13.1893310470
H	8.7313293256	5.7609362816	4.8264415459	H	4.3261414908	10.2983949374	13.6607681284
C	6.8929223804	6.9016660872	7.8671449987	H	3.5144326808	11.8184770886	13.18124617
H	6.9718756784	6.1686061095	8.6899802863				
C	12.3160384161	5.0918837482	13.3341250661				
H	13.2239889646	5.3119942776	13.9136503780				
H	12.3011513731	4.0075961628	13.1218115450				
N	14.6665663611	9.4169126152	6.8696666770				
N	12.9149672649	13.2047844262	14.2286760710				
N	13.5970555194	14.6684600870	11.7933076687				
N	14.3362961133	12.3723139208	7.1713673426				
C	11.5685107456	11.2183264517	13.9305949561				
C	10.3369228136	11.9085052822	13.9461777186				
H	10.3556564280	12.9950740994	13.9700943602				
C	13.0863175823	12.5495719688	6.9730500710				
H	12.5953151962	12.2391036332	6.0329626575				
C	12.2143251470	13.2130880971	7.9626846816				
C	12.6959536242	13.5645852182	9.2358028623				
H	13.7205389027	13.3339843246	9.5055587633				
C	12.8428861102	11.9669079383	13.9155299198				
H	13.7306576098	11.3936869821	13.5929902450				
C	12.3618219414	14.6942863458	11.4592898379				
H	11.5904405391	15.1023432875	12.1366116320				
C	15.7251413830	10.4080464011	6.6806396324				
H	16.4258578054	10.0116372778	5.9334224142				
H	16.2831391457	10.6254671142	7.6079603841				
C	14.1844713077	13.9117700196	14.0625197218				
H	14.9844231287	13.2742341800	13.6478001346				
H	14.5067344835	14.2865311914	15.0436735231				
C	10.5415237565	14.5240985884	9.7818947361				
H	9.8914802811	15.0379558108	10.4890338604				
C	10.9042549684	13.5547729001	7.5987785014				
H	10.5260080631	13.3236521126	6.6062113067				
C	10.0617438377	14.2235588031	8.5014248256				
C	11.8682609212	14.2307044559	10.1481455828				
C	15.1274732539	11.7211245596	6.1322574010				
H	15.9564930239	12.3928853459	5.8704708474				
H	14.5487789073	11.5065035386	5.2163120854				
C	14.4136969025	9.0142412090	8.0568578970				
H	14.9957905872	9.3659416724	8.9275035078				
C	13.9489769463	15.1313442927	13.1348159712				
H	13.1667209847	15.7666518135	13.5849154405				
H	14.8790678045	15.7097482351	13.0694393976				
N	8.3571100874	14.7620761898	6.8865756334				
N	6.7264184207	11.3428589854	14.1374664829				
N	4.9474020539	11.1866922749	11.8095459752				
N	5.9985898415	12.9357086691	7.0203520233				

