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Supplementary Material for:

The fine balance between one cross-coupling and two β-hydride elimination pathways: A DFT mechanistic study of Ni(π-allyl)2-catalyzed cross-coupling of alkyl halides and alkyl Grignard reagents

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1. Supplementary Methods and References

Methods

Quantum Chemical Calculations

Theoretical investigations were carried out with electronic structure computations, using the Becke-3-Lee-Yang-Parr (B3LYP) [1] Density Functional Theory (DFT) method combined with the Self Consistent Reaction Field Polar Continuum Model (SCRF-PCM) [2] implicit solvent approach, employing the all-electron DZVP basis set[3] for all atoms, using the Gaussian03 (G03) program package.[4] Bader-determined radii were used for all atoms. All transition state (TS) structures were located using numeric and manual means, based on a standardised methodology.[5]. All structures were confirmed by frequency calculations as residing at minima or 1st order TSs, on their respective potential energy hypersurfaces (PEHSs) To ensure quantitative characterisation of all intra-molecular interactions, Bader's Atoms-In-Molecules (AIM) analyses were conducted on the wavefunctions generated from the B3LYP/DZVP geometry-optimised structures..

Atoms-In-Molecules (AIM)

Bader's Atoms-In-Molecules analyses were performed using the AIM2000 program package [6], using default values. The topological properties of the electron density distribution $\rho(r)$ of a molecule are based on the gradient vector field of the electron density $\nabla\rho(r)$, and on the Laplacian of the electron density $\nabla^2\rho(r)$, where r is the positional vector in three-dimensional (3D) space. In view of the AIM approach [7], critical points (CPs) of rank 3 were identified in the electron densities, which include bond, ring and cage critical points (BCPs, RCPs and CCPs, respectively). The pairs of gradient paths that originate at a BCP and terminate at neighbouring nuclei define a line through which $\rho(r)$ is a maximum with respect to any lateral displacement. Relevant bond and interaction strengths are directly comparable through their respective ρ_b-values, defined as the number of electrons N_e per spherical Bohr-volume V_B ($N_eV_B^{-3}$). The ρ_b-values are a comparable quantitative measure for identical pairs of atoms. A region of space Ω is bound by a surface satisfying the condition of zero-flux in the gradient vector field of the charge density, $\nabla\rho(r)\circ n(r)=0$, with $n(r)$ being the normal to surface unit vector. The region of space Ω is employed for integrating the electron population and energy of atom in a molecule, $N(\Omega)=\int_\Omega \rho(r)d\tau$ and $E_e(\Omega)=\int_\Omega E_e(r)d\tau$.[8]

Supplementary Material Structures

All geometric structure visualisations contained in the supplementary material were generated using the Molekel 4.3 program package. [9]

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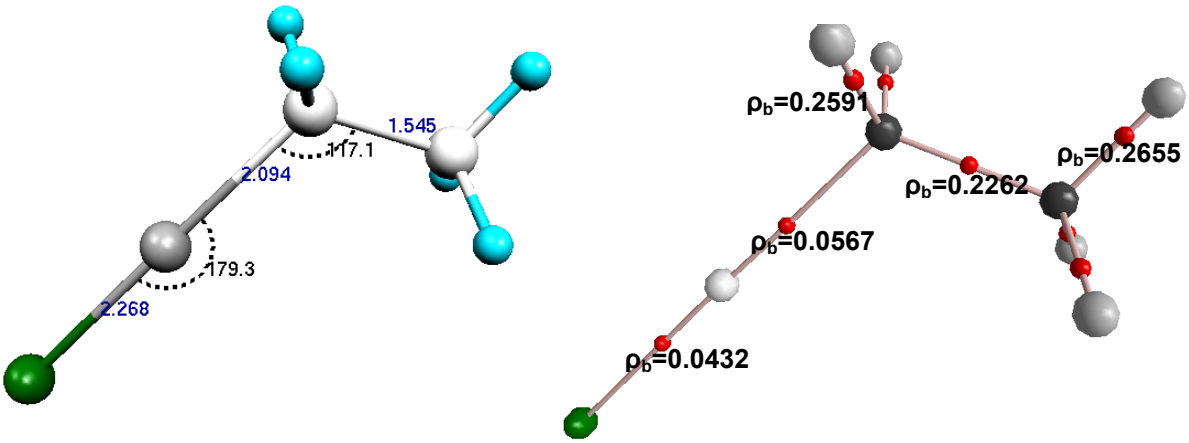
2. Schematic Illustrations of Structures and Molecular Graphs

The following geometric structures have been visualised using the Molekel 4.3 program package. H, C, N, Cl and Pd atoms are represented by white, cyan, blue, green and grey spheres, respectively. Weakly polar interactions (as determined by AIM analyses) are represented by red dashed lines, and include the inter-atomic distances, in angstroms (Å).

Molecular graphs of wavefunctions from B3LYP/DZVP geometry-optimised structures show all intra-molecular bonding and interactions. Light grey, dark grey, white, green, off-white and off-white spheres represent H, C, Mg, Cl, Ni, and Br atoms, respectively. Red and yellow dots represent BCPs and RCPs, respectively. Selected ρ_b-values (ē•bohr^3) are provided for the BCP closest to the '=' or decimal point of each value, or as indicated by an arrow. These values are in no-way comparable for non-identical atom pairs, not even qualitatively. Some atoms are visually truncated for clarity.

C_2H_5MgCl



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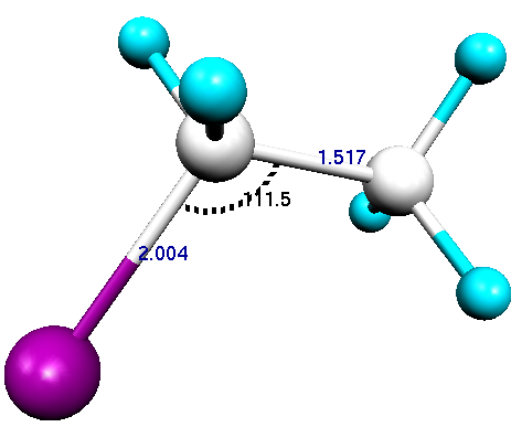
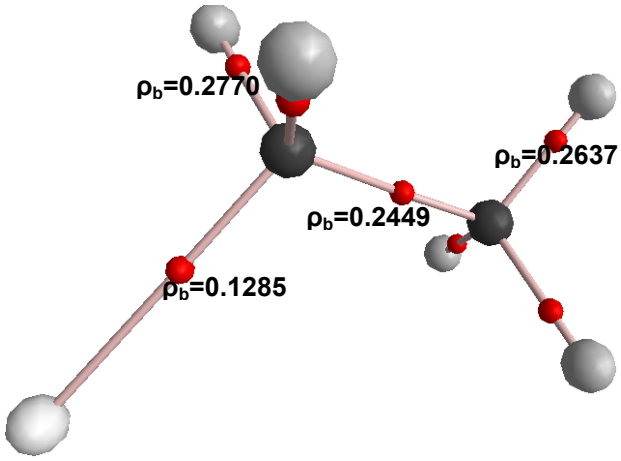
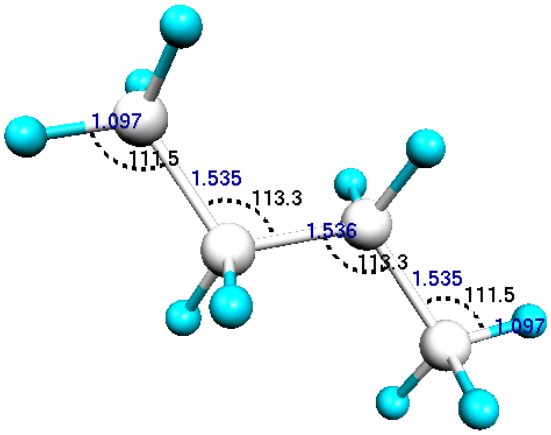
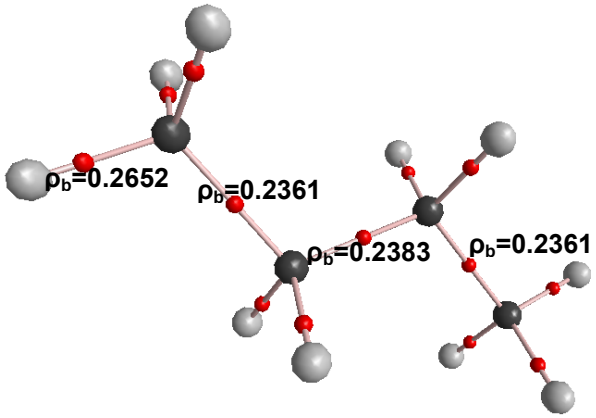
C_2H_5Br



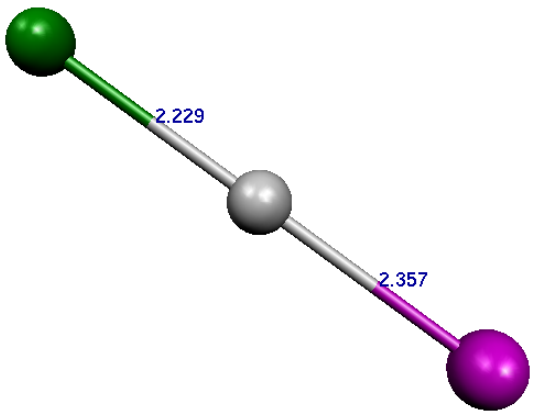


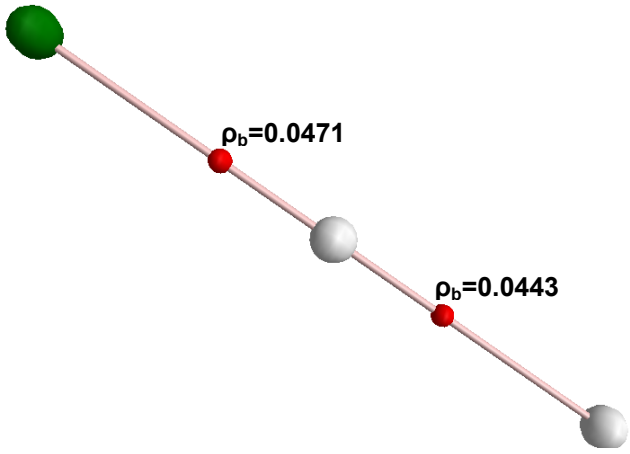
$n\text{-}C_4H_{10}$ (all-*anti* conformation)





Mg-Br-Cl





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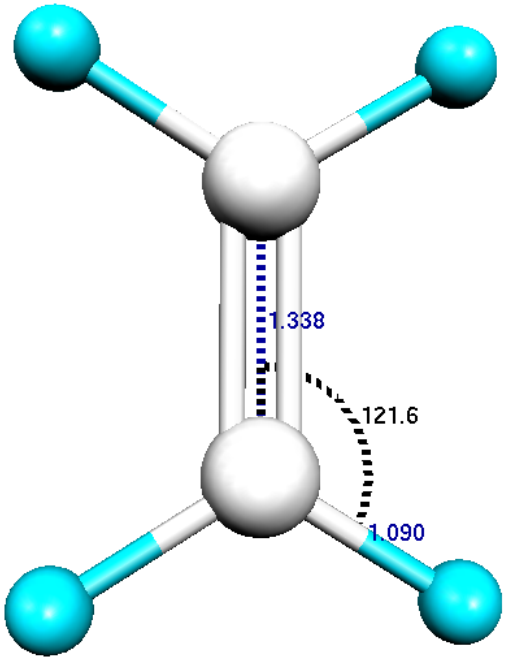
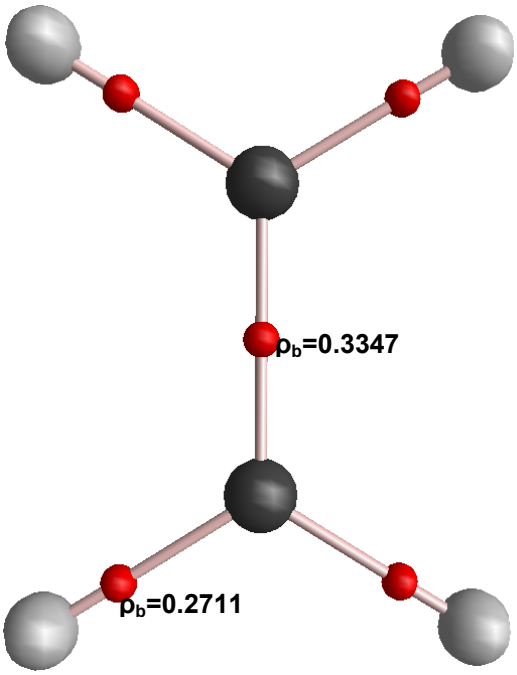
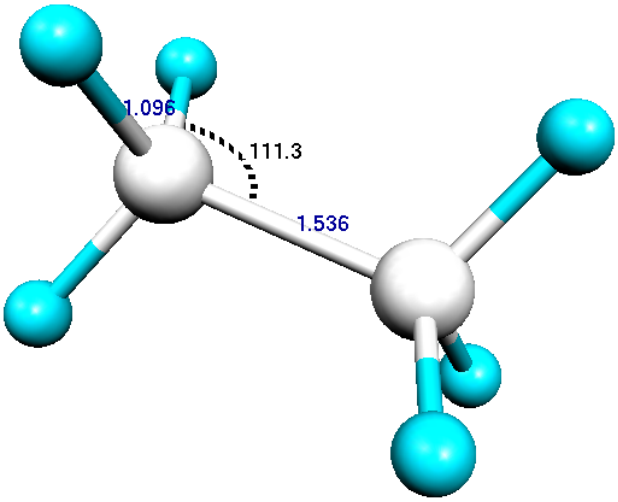
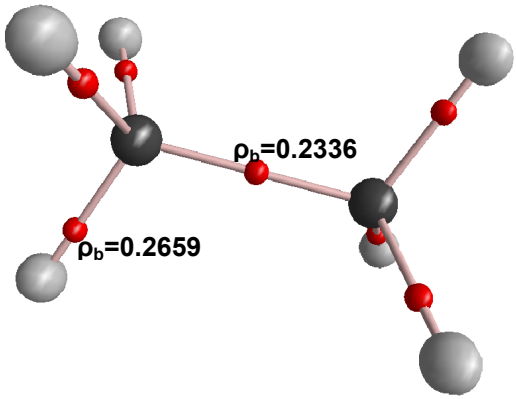
Ethene





Ethane (eclipsed)





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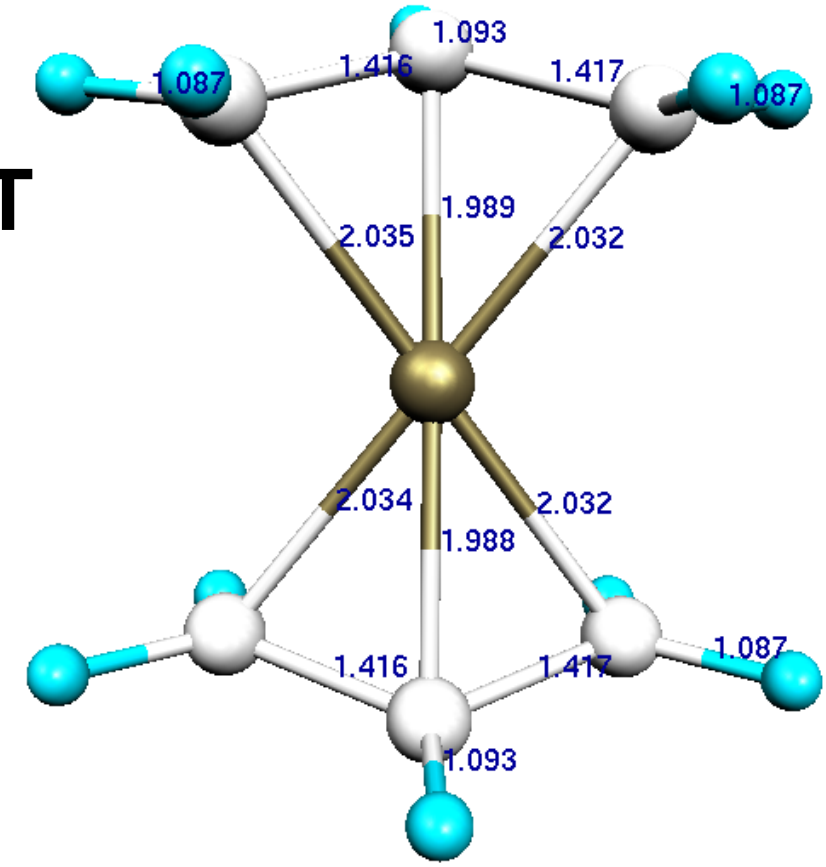
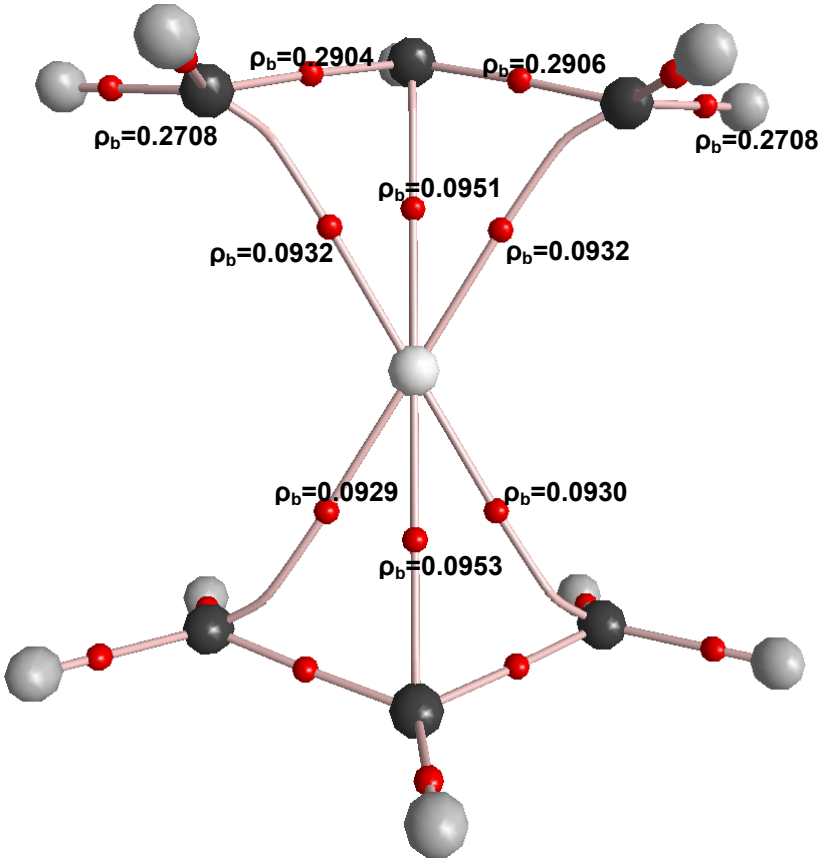
CAT





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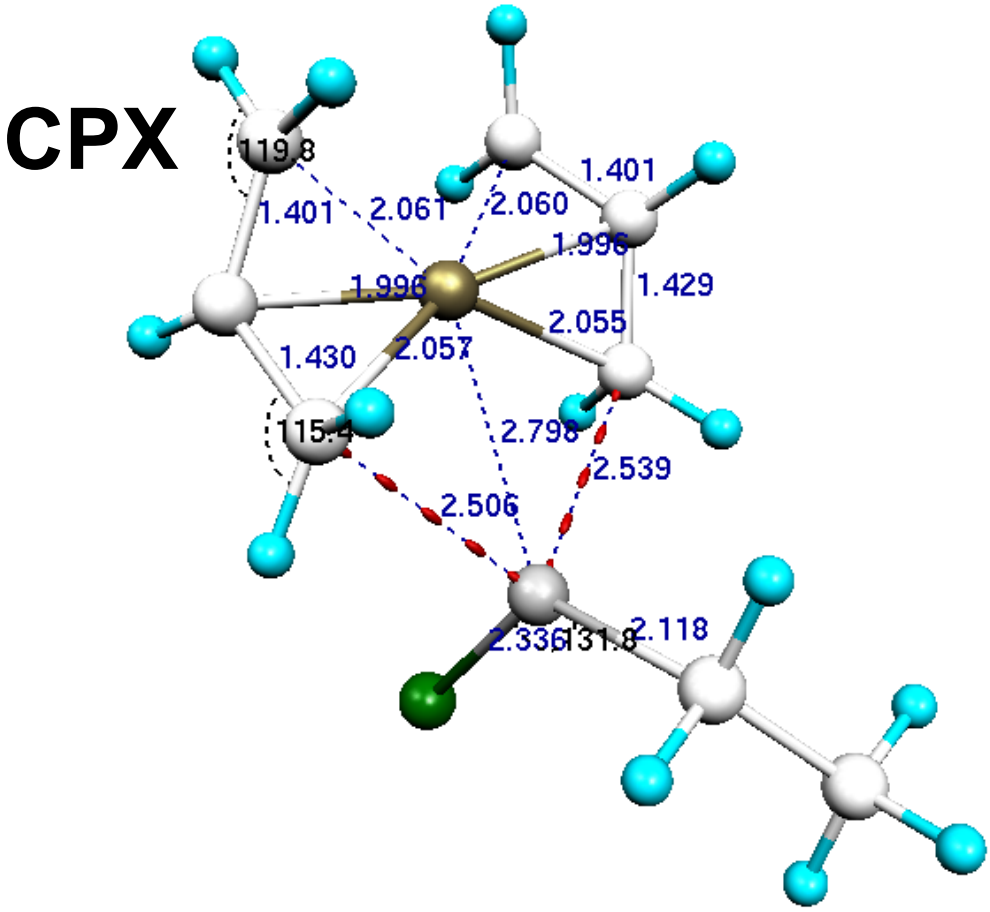

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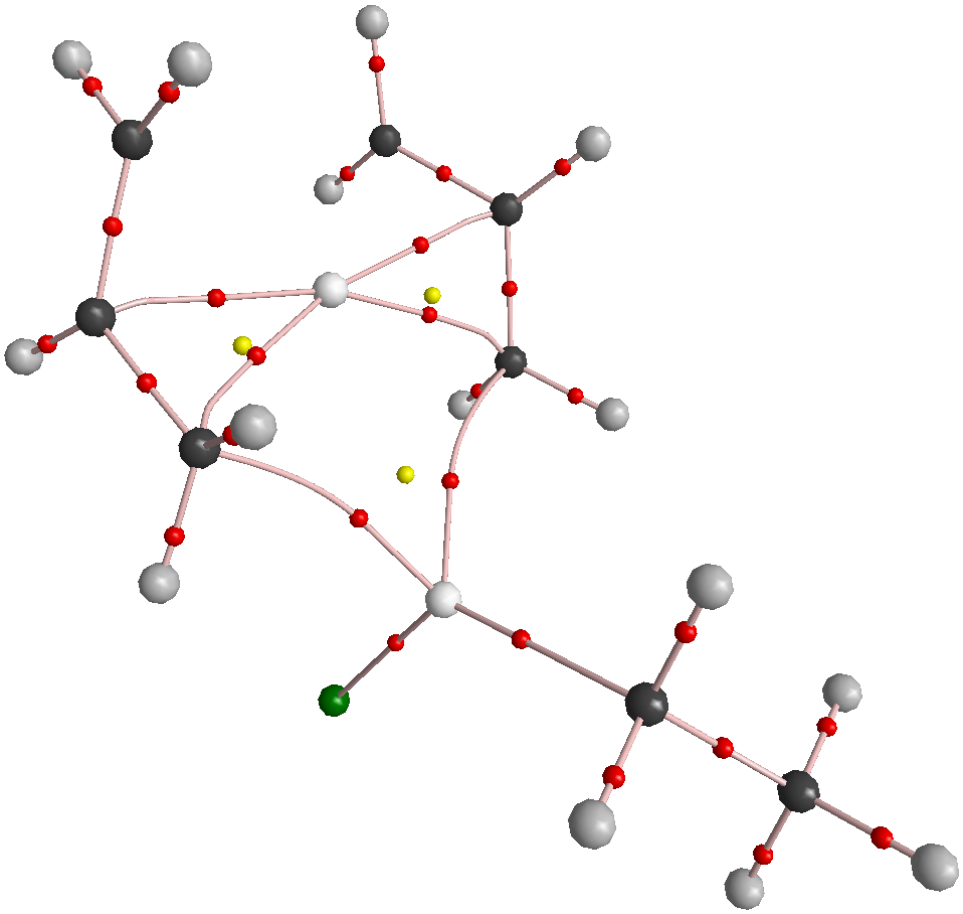

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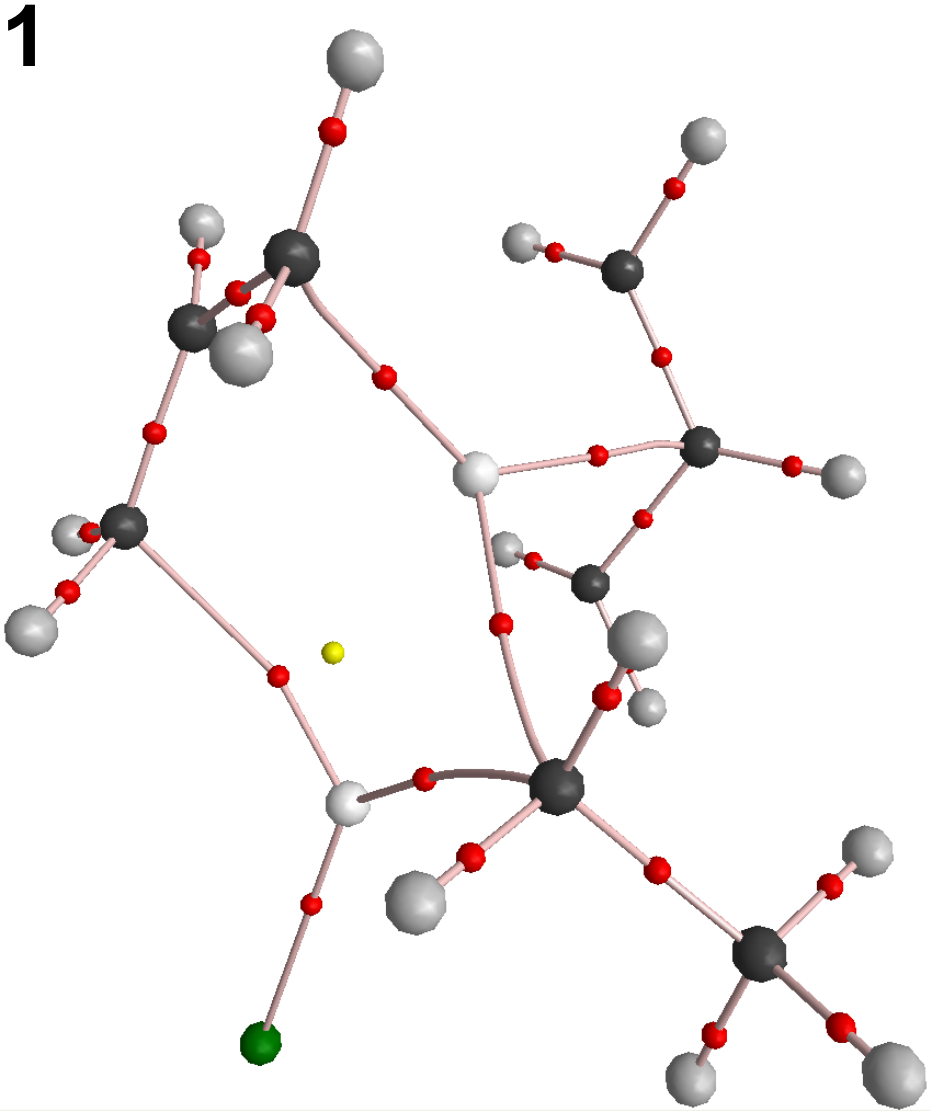

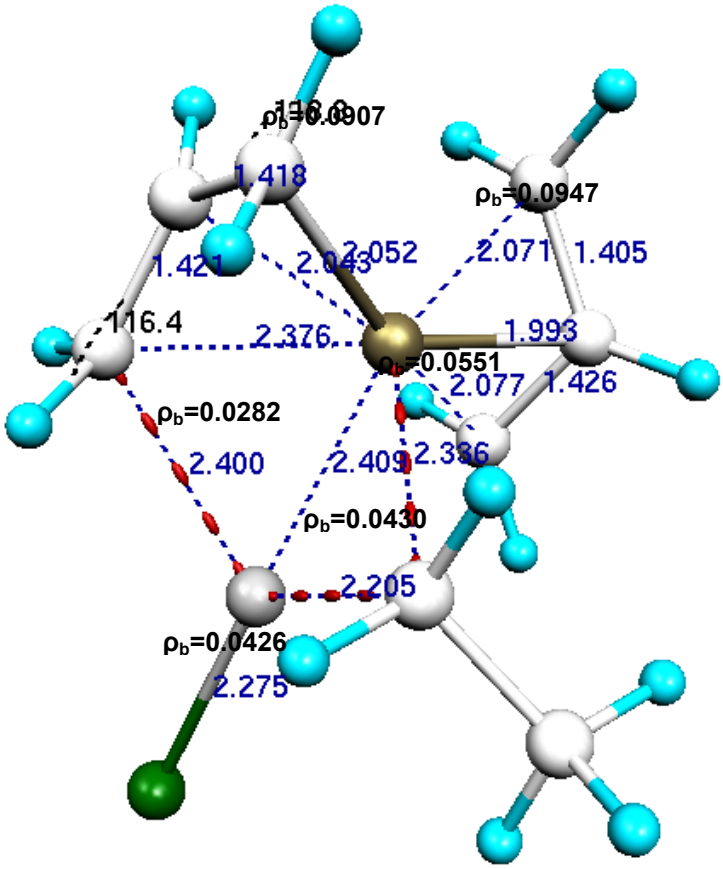

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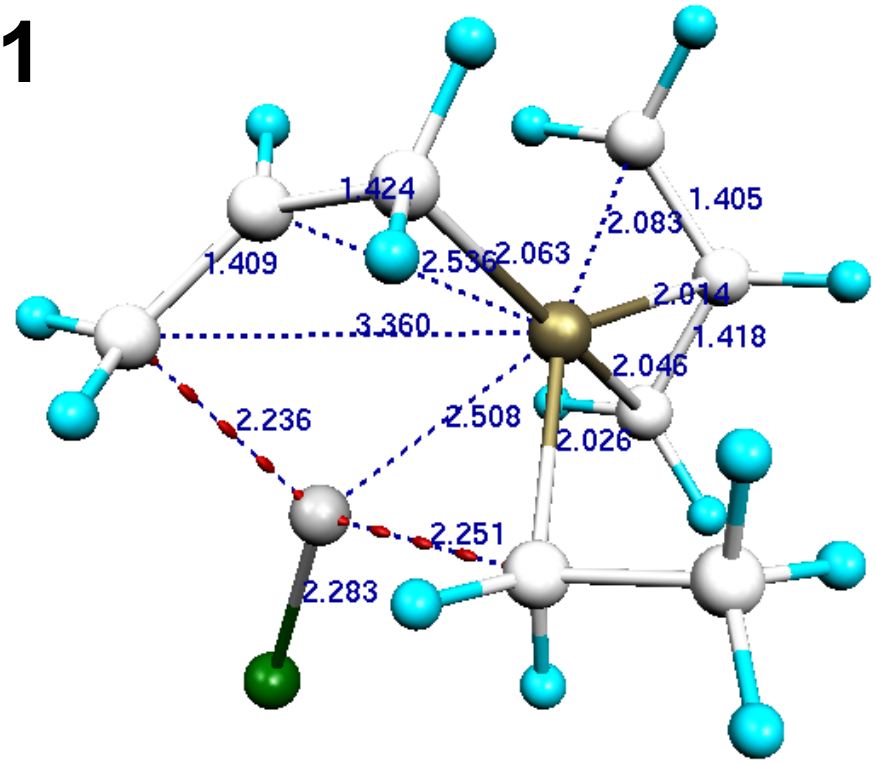

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ρ_b=0.0916

ρ_b=0.0373 **ρ_b=0.0916**

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ρ_b=0.0414

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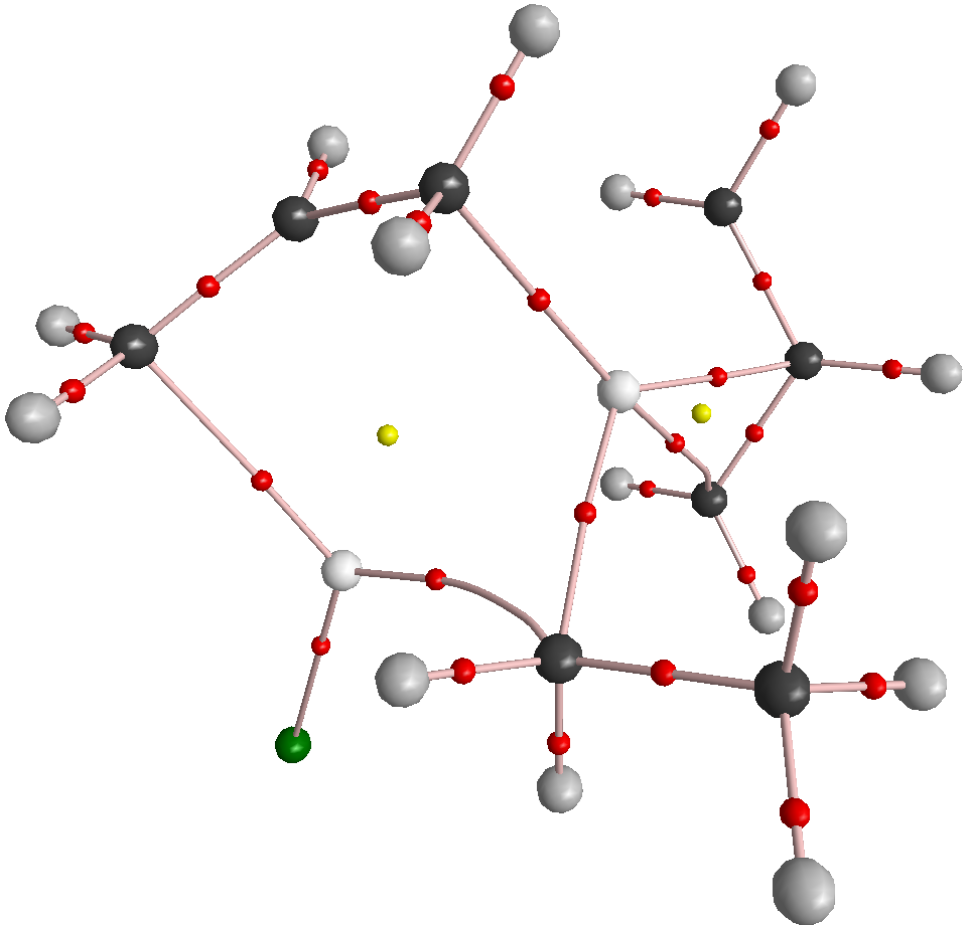

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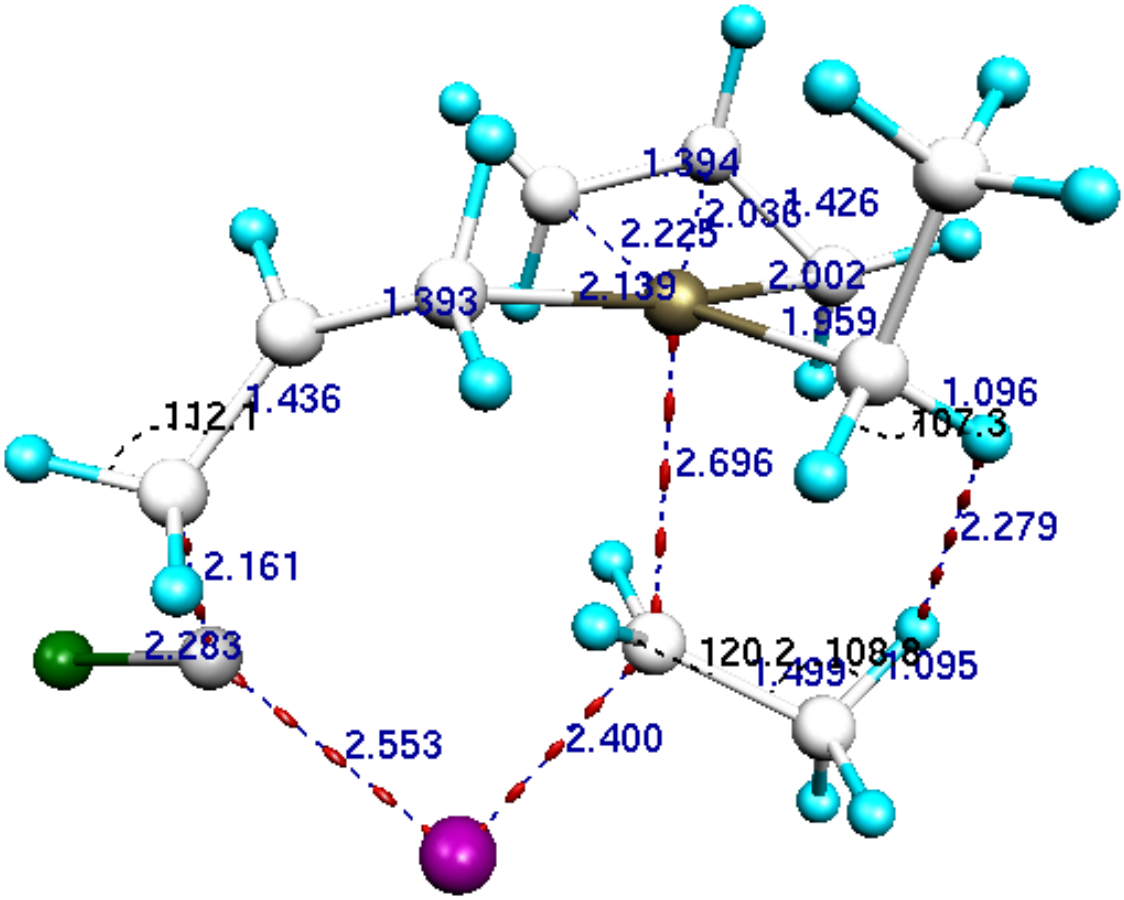

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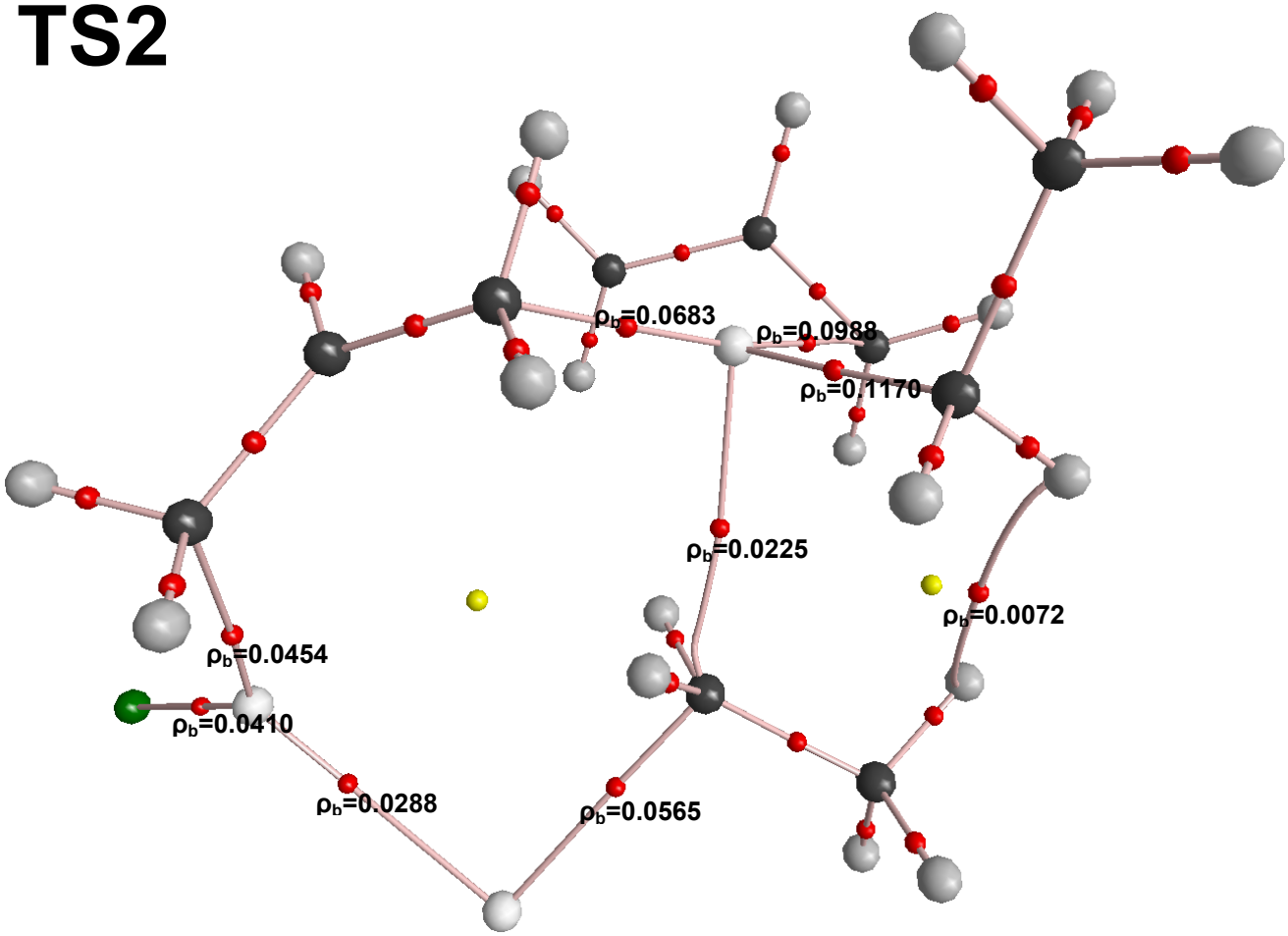

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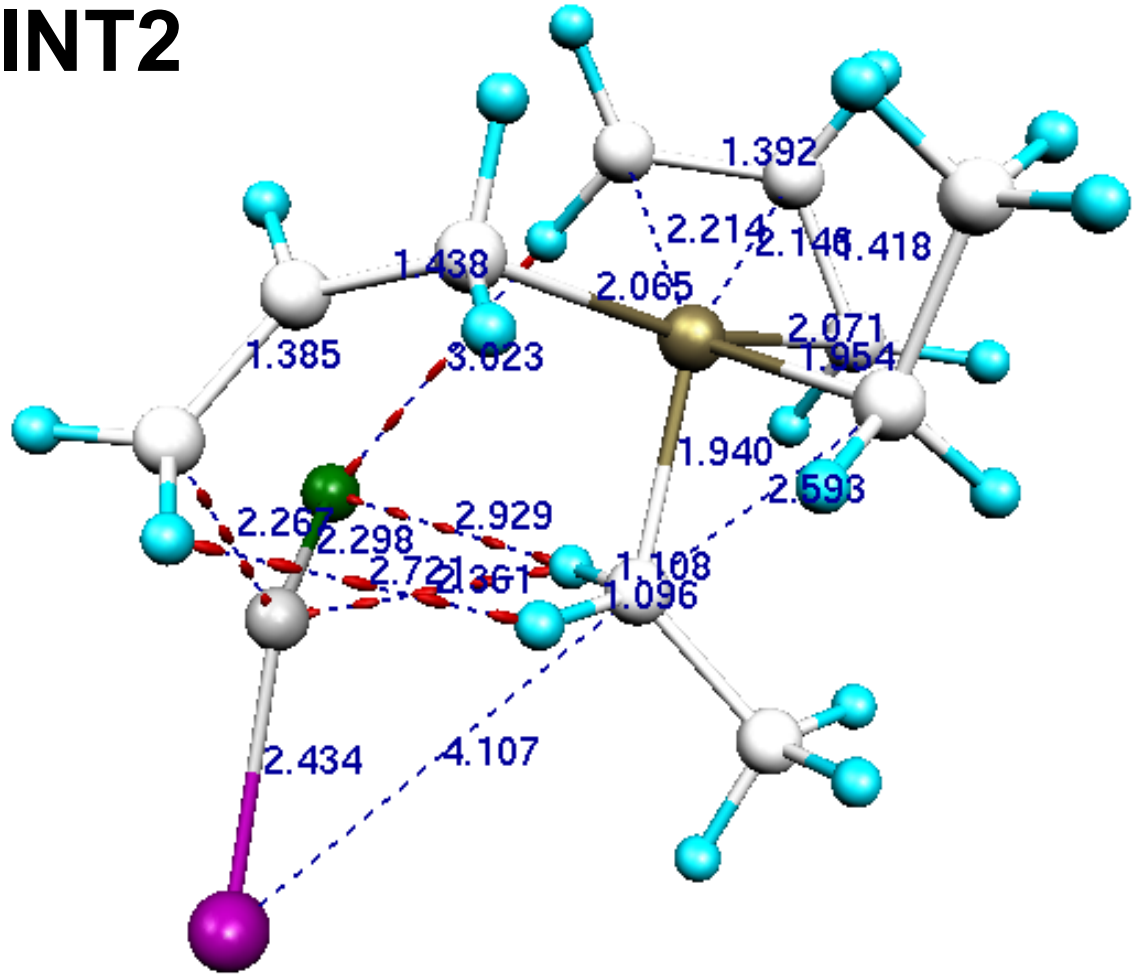

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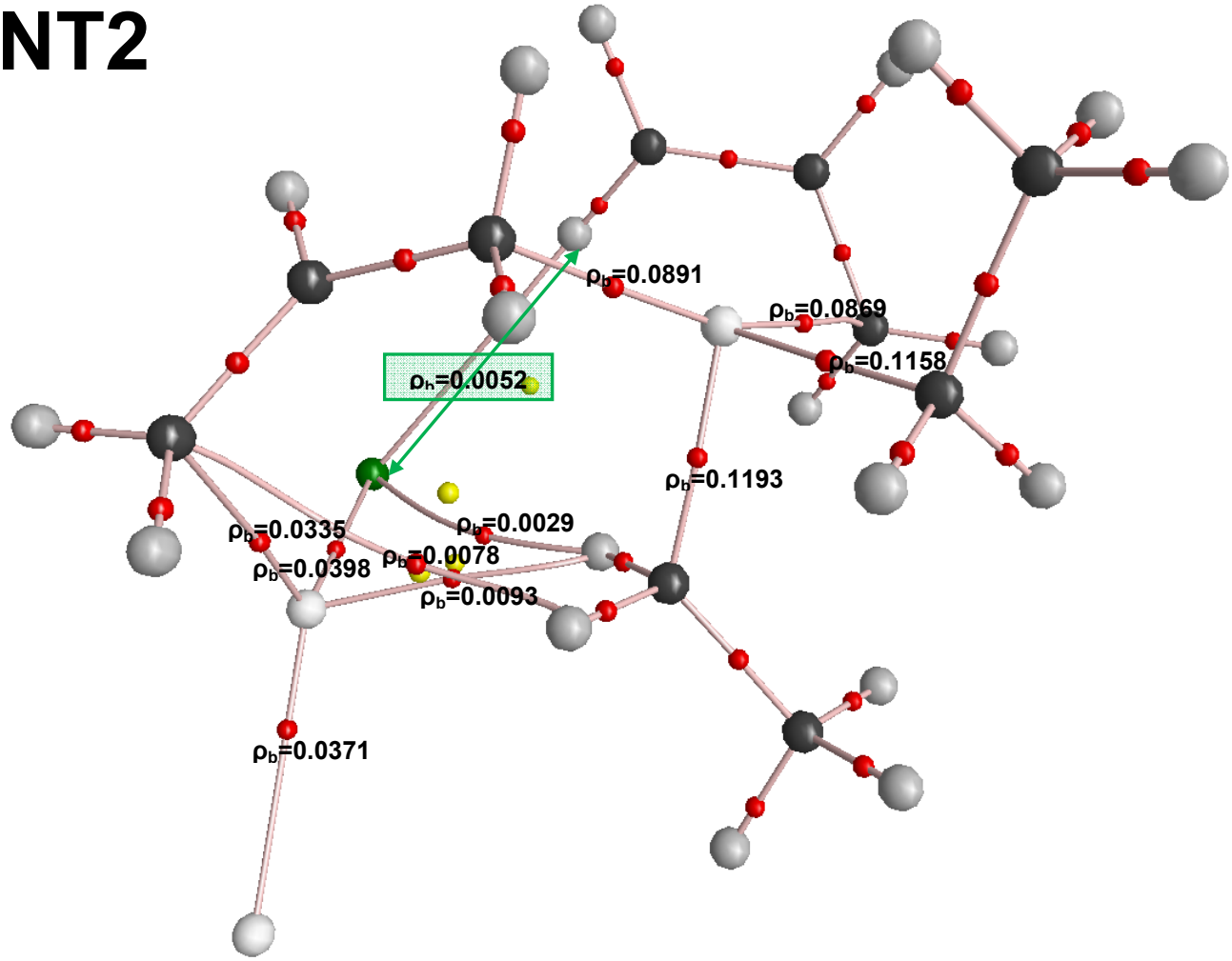

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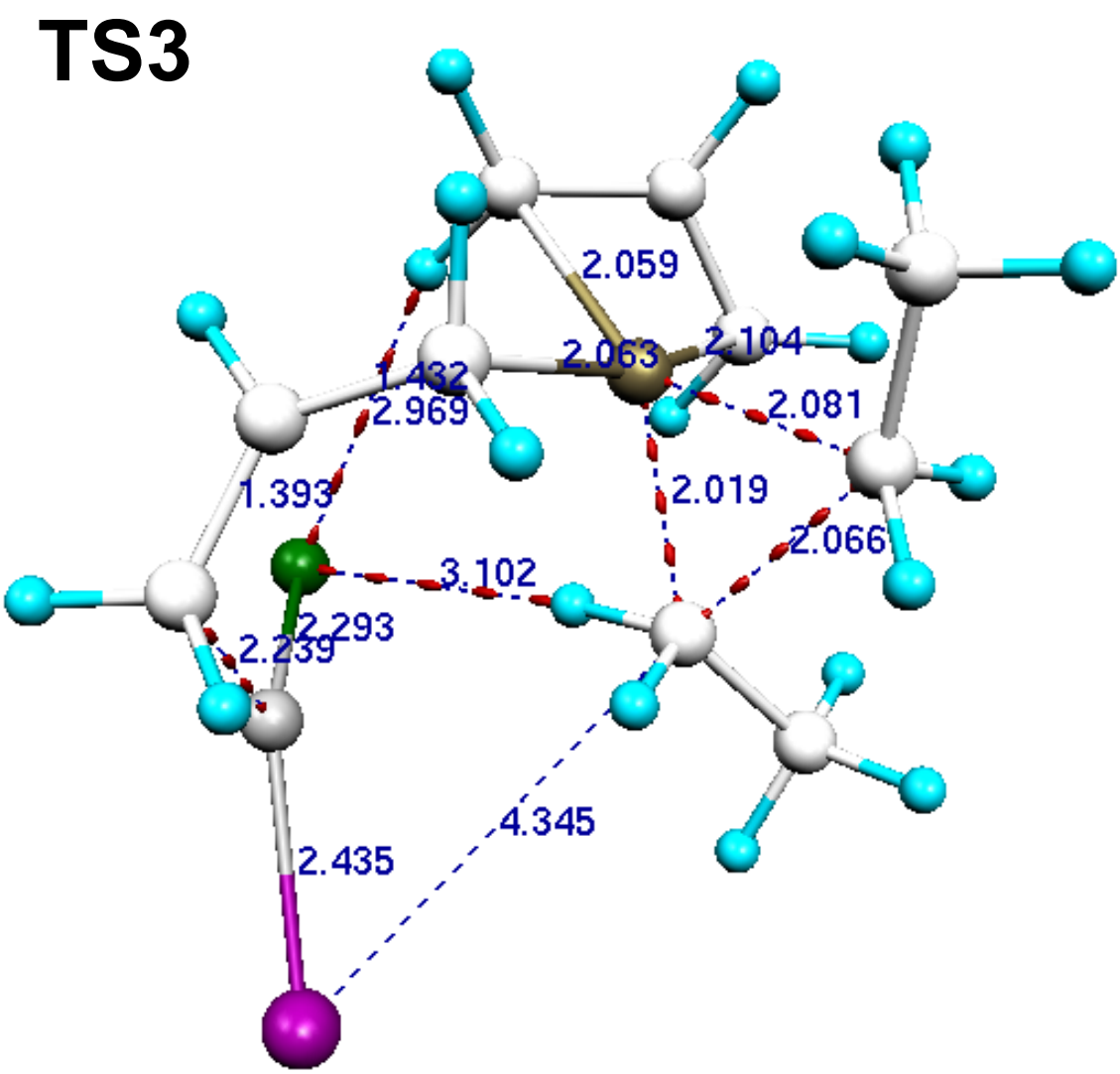

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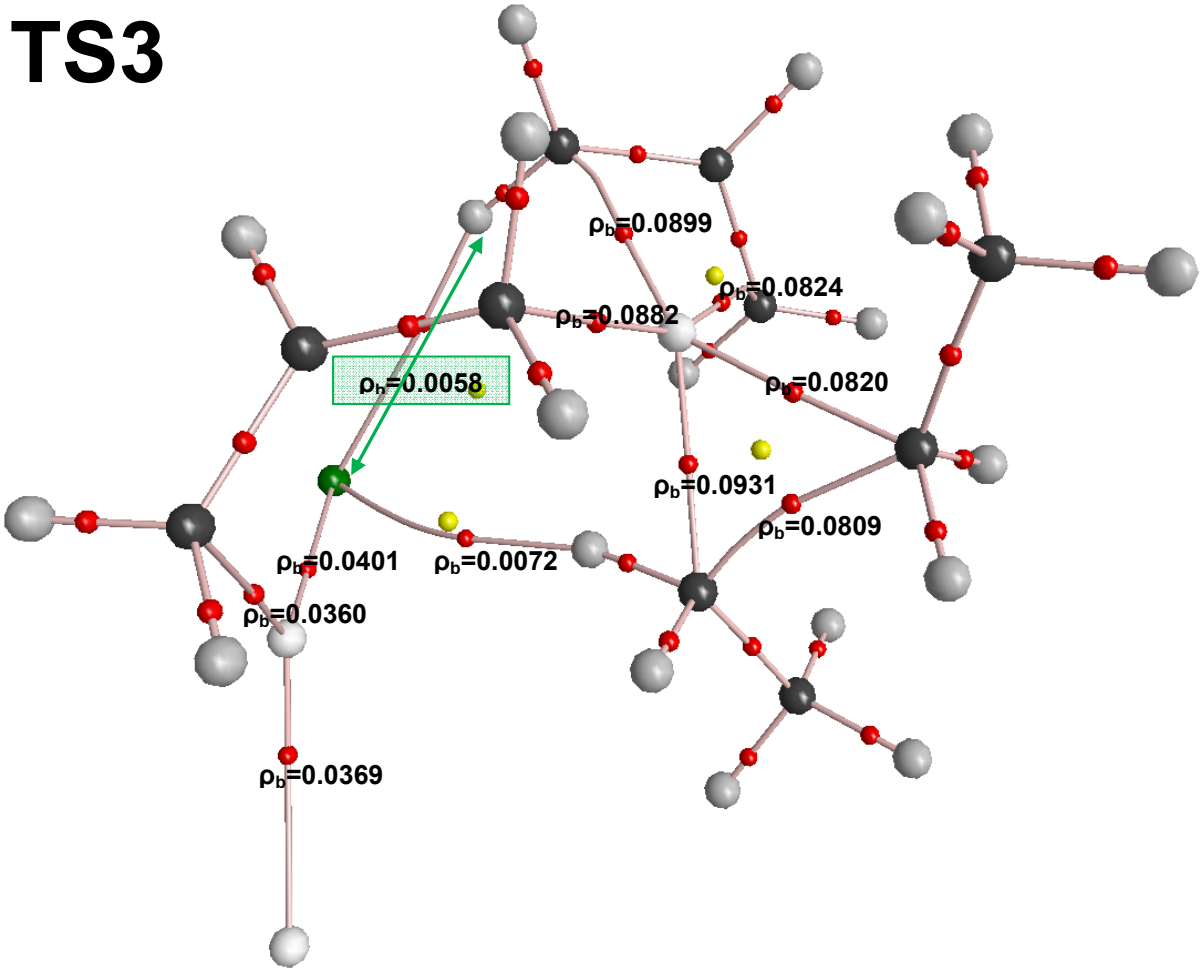

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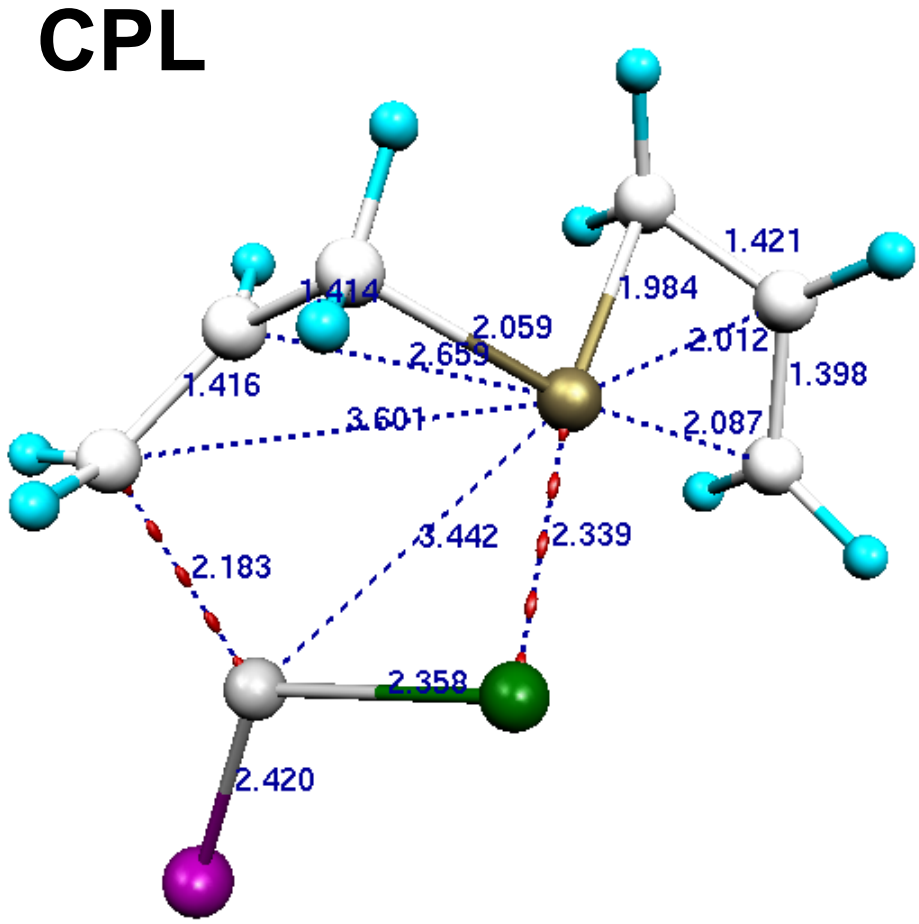

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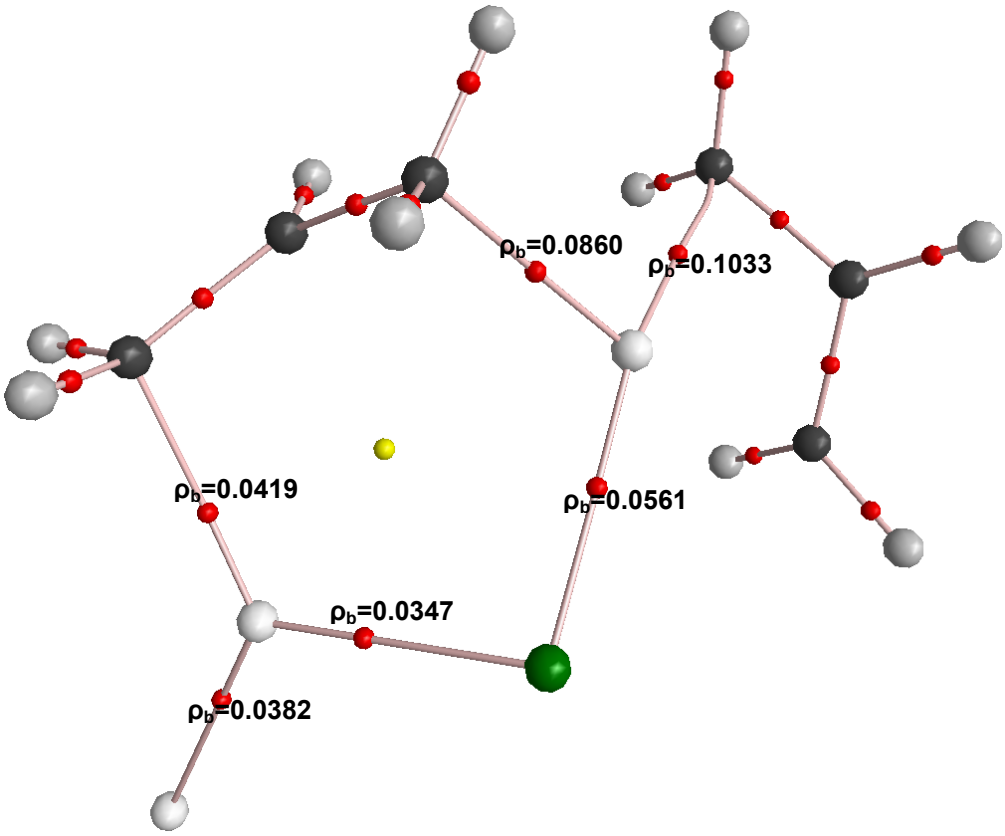

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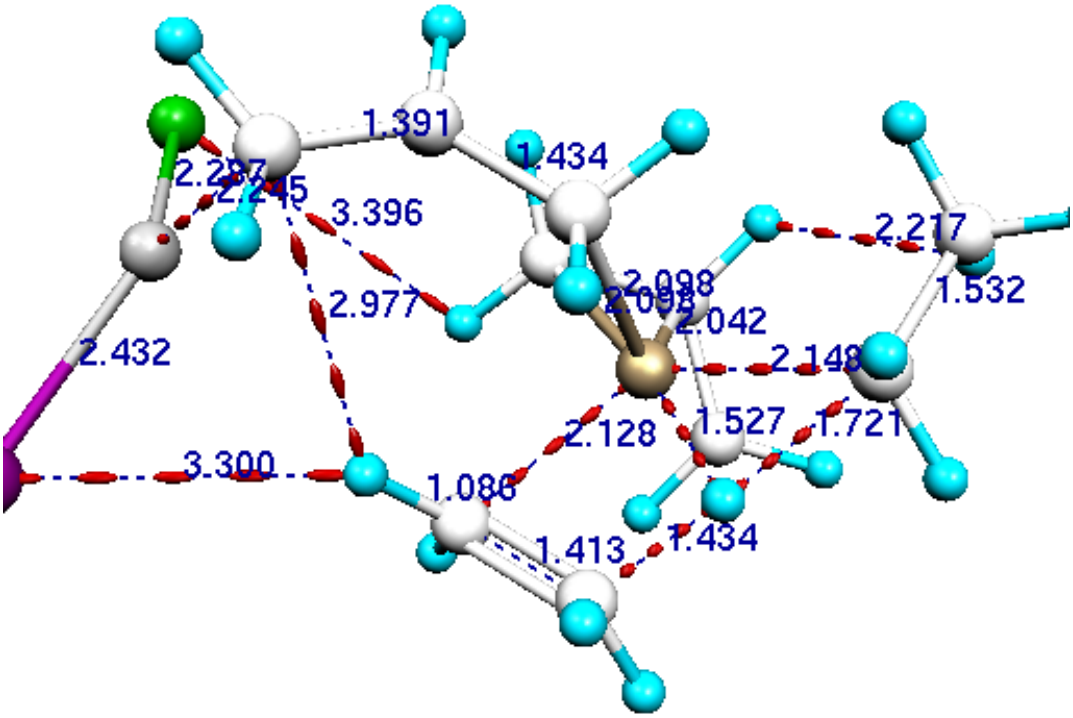
TS β-H (1)



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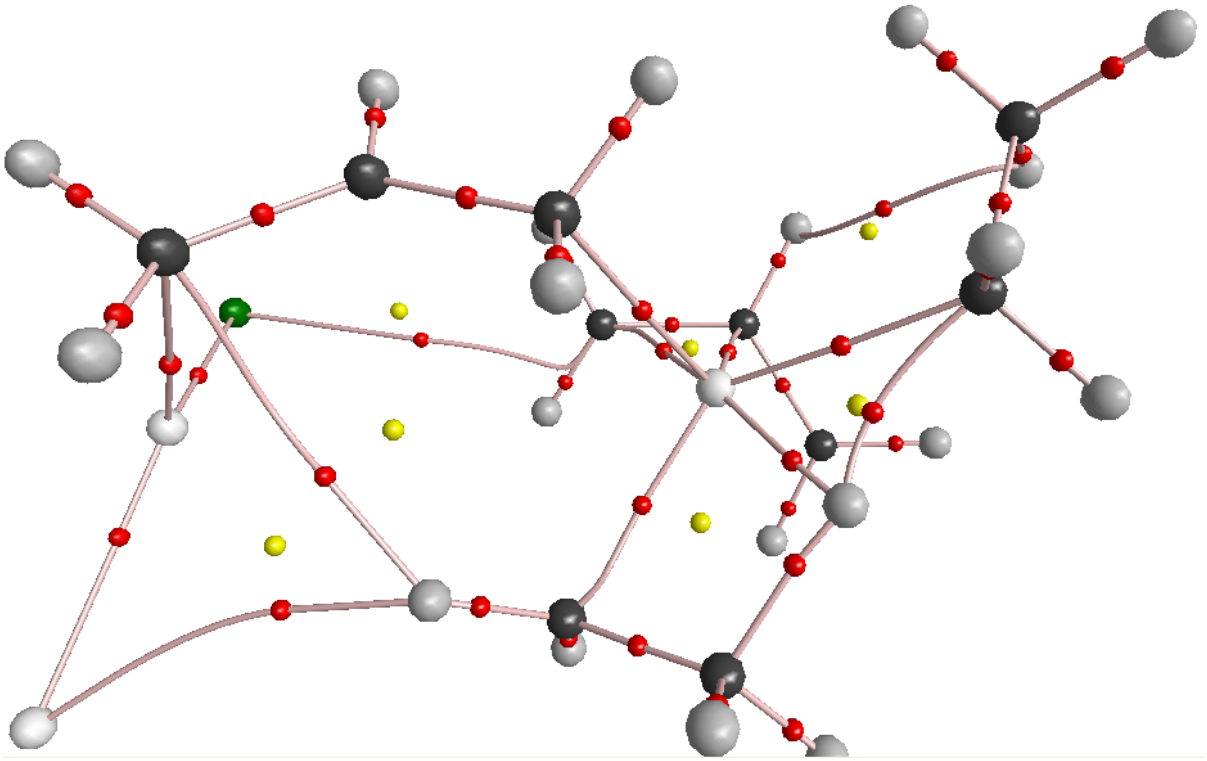

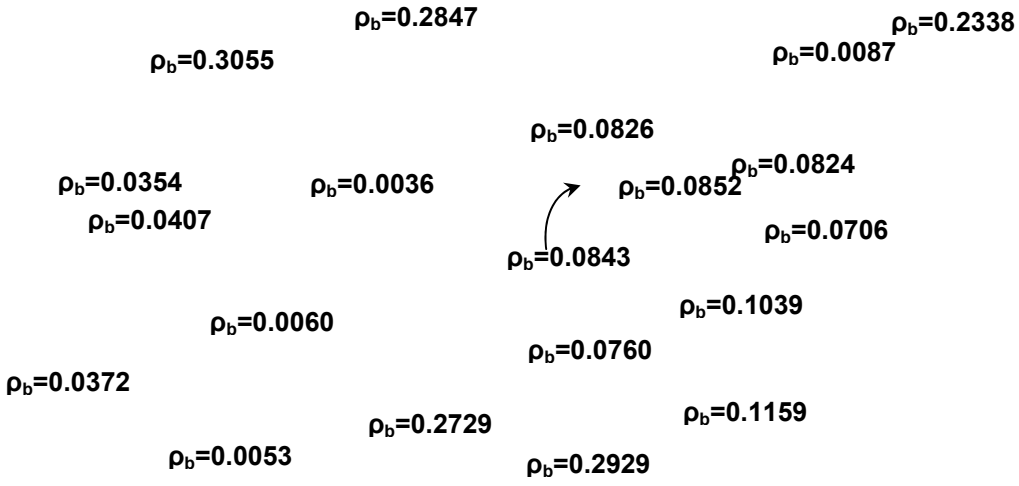

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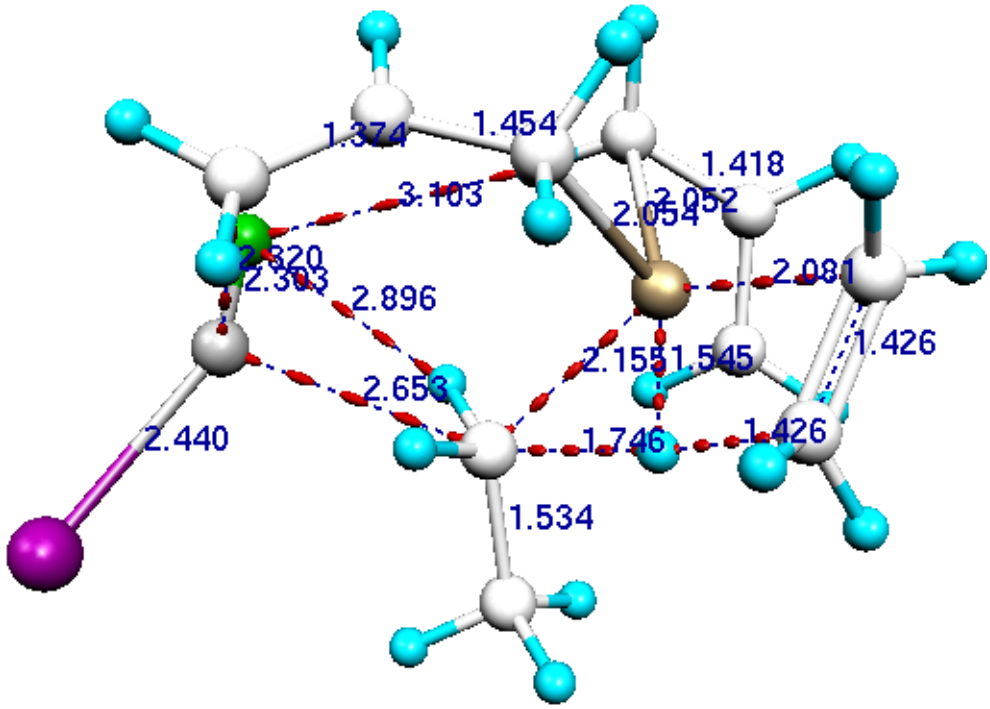

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ρ_b=0.2858

ρ_b=0.0289

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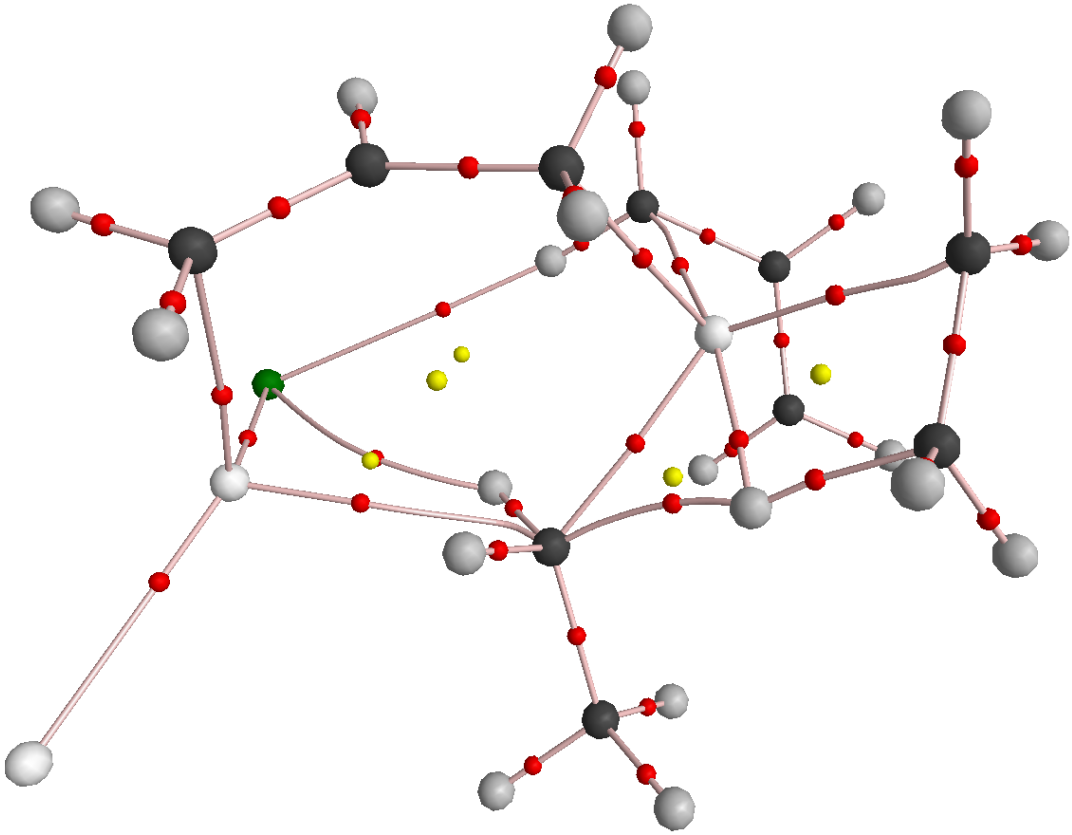

3. Thermodynamic Parameters of Geometry-Optimised Structures

C_2H_5MgCl

Zero-point correction= 0.064764 (Hartree/Particle)
Thermal correction to Energy= 0.069621
Thermal correction to Enthalpy= 0.070391
Thermal correction to Gibbs Free Energy= 0.040441
Sum of electronic and zero-point Energies= -739.481936
Sum of electronic and thermal Energies= -739.477079
Sum of electronic and thermal Enthalpies= -739.476309
Sum of electronic and thermal Free Energies= -739.506259

C_2H_5Br

Zero-point correction= 0.065962 (Hartree/Particle)
Thermal correction to Energy= 0.069087
Thermal correction to Enthalpy= 0.069857
Thermal correction to Gibbs Free Energy= 0.044402
Sum of electronic and zero-point Energies= -2652.869219
Sum of electronic and thermal Energies= -2652.866095
Sum of electronic and thermal Enthalpies= -2652.865325
Sum of electronic and thermal Free Energies= -2652.890780

n-C_4H_{10} (all *anti*)

Zero-point correction= 0.131914 (Hartree/Particle)
Thermal correction to Energy= 0.136116

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Thermal correction to Enthalpy= 0.136886
Thermal correction to Gibbs Free Energy= 0.110664
Sum of electronic and zero-point Energies= -158.345181
Sum of electronic and thermal Energies= -158.340979
Sum of electronic and thermal Enthalpies= -158.340210
Sum of electronic and thermal Free Energies= -158.366431

Mg-Br-Cl

Zero-point correction= 0.001898 (Hartree/Particle)
Thermal correction to Energy= 0.005660
Thermal correction to Enthalpy= 0.006430
Thermal correction to Gibbs Free Energy= -0.020808
Sum of electronic and zero-point Energies= -3234.091949
Sum of electronic and thermal Energies= -3234.088186
Sum of electronic and thermal Enthalpies= -3234.087417
Sum of electronic and thermal Free Energies= -3234.114655

Ethene

Zero-point correction= 0.050680 (Hartree/Particle)
Thermal correction to Energy= 0.053064
Thermal correction to Enthalpy= 0.053834
Thermal correction to Gibbs Free Energy= 0.034309
Sum of electronic and zero-point Energies= -78.548911
Sum of electronic and thermal Energies= -78.546527
Sum of electronic and thermal Enthalpies= -78.545758
Sum of electronic and thermal Free Energies= -78.565282

Ethane

Zero-point correction= 0.074696 (Hartree/Particle)
Thermal correction to Energy= 0.077364
Thermal correction to Enthalpy= 0.078134
Thermal correction to Gibbs Free Energy= 0.057944
Sum of electronic and zero-point Energies= -79.766059
Sum of electronic and thermal Energies= -79.763392
Sum of electronic and thermal Enthalpies= -79.762622
Sum of electronic and thermal Free Energies= -79.782812

CAT

Zero-point correction= 0.139998 (Hartree/Particle)
Thermal correction to Energy= 0.145710
Thermal correction to Enthalpy= 0.146480
Thermal correction to Gibbs Free Energy= 0.115077
Sum of electronic and zero-point Energies= -1742.609072
Sum of electronic and thermal Energies= -1742.603360
Sum of electronic and thermal Enthalpies= -1742.602590
Sum of electronic and thermal Free Energies= -1742.633993

CPX

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Zero-point correction= 0.206676 (Hartree/Particle)
Thermal correction to Energy= 0.218441
Thermal correction to Enthalpy= 0.219210
Thermal correction to Gibbs Free Energy= 0.170107
Sum of electronic and zero-point Energies= -2482.107870
Sum of electronic and thermal Energies= -2482.096106
Sum of electronic and thermal Enthalpies= -2482.095336
Sum of electronic and thermal Free Energies= -2482.144439

TS1

Zero-point correction= 0.206158 (Hartree/Particle)
Thermal correction to Energy= 0.217034
Thermal correction to Enthalpy= 0.217803
Thermal correction to Gibbs Free Energy= 0.173901
Sum of electronic and zero-point Energies= -2482.088504
Sum of electronic and thermal Energies= -2482.077629
Sum of electronic and thermal Enthalpies= -2482.076859
Sum of electronic and thermal Free Energies= -2482.120761

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INT1

Zero-point correction= 0.206764 (Hartree/Particle)
Thermal correction to Energy= 0.218184
Thermal correction to Enthalpy= 0.218953
Thermal correction to Gibbs Free Energy= 0.173198
Sum of electronic and zero-point Energies= -2482.103475
Sum of electronic and thermal Energies= -2482.092055
Sum of electronic and thermal Enthalpies= -2482.091285
Sum of electronic and thermal Free Energies= -2482.137040

TS2

Zero-point correction= 0.271282 (Hartree/Particle)
Thermal correction to Energy= 0.287313
Thermal correction to Enthalpy= 0.288083
Thermal correction to Gibbs Free Energy= 0.230101
Sum of electronic and zero-point Energies= -5134.934069
Sum of electronic and thermal Energies= -5134.918037
Sum of electronic and thermal Enthalpies= -5134.917267
Sum of electronic and thermal Free Energies= -5134.975250

INT2

Zero-point correction= 0.274060 (Hartree/Particle)
Thermal correction to Energy= 0.289785
Thermal correction to Enthalpy= 0.290554
Thermal correction to Gibbs Free Energy= 0.234047
Sum of electronic and zero-point Energies= -5134.983635
Sum of electronic and thermal Energies= -5134.967911
Sum of electronic and thermal Enthalpies= -5134.967141
Sum of electronic and thermal Free Energies= -5135.023648

TS3

Zero-point correction= 0.274893 (Hartree/Particle)
Thermal correction to Energy= 0.289925
Thermal correction to Enthalpy= 0.290694
Thermal correction to Gibbs Free Energy= 0.235278
Sum of electronic and zero-point Energies= -5134.974491
Sum of electronic and thermal Energies= -5134.959459
Sum of electronic and thermal Enthalpies= -5134.958690
Sum of electronic and thermal Free Energies= -5135.014106

CPL

Zero-point correction= 0.142989 (Hartree/Particle)
Thermal correction to Energy= 0.153391
Thermal correction to Enthalpy= 0.154160
Thermal correction to Gibbs Free Energy= 0.108256
Sum of electronic and zero-point Energies= -4976.711931
Sum of electronic and thermal Energies= -4976.701529
Sum of electronic and thermal Enthalpies= -4976.700759

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Sum of electronic and thermal Free Energies= -4976.746664

TS β-H (1)

Zero-point correction= 0.269780 (Hartree/Particle)
Thermal correction to Energy= 0.284396
Thermal correction to Enthalpy= 0.285166
Thermal correction to Gibbs Free Energy= 0.231834
Sum of electronic and zero-point Energies= -5134.937679
Sum of electronic and thermal Energies= -5134.923063
Sum of electronic and thermal Enthalpies= -5134.922294
Sum of electronic and thermal Free Energies= -5134.975625

TS β-H (2)

Zero-point correction= 0.270795 (Hartree/Particle)
Thermal correction to Energy= 0.285665
Thermal correction to Enthalpy= 0.286435
Thermal correction to Gibbs Free Energy= 0.232664
Sum of electronic and zero-point Energies= -5134.947779
Sum of electronic and thermal Energies= -5134.932909
Sum of electronic and thermal Enthalpies= -5134.932139
Sum of electronic and thermal Free Energies= -5134.985910

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4. Normal Modes of Vibration (within computational error of ±25 cm^{-1})

C_2H_5MgCl

Frequencies --	51.2503	71.8348	206.3969
Frequencies --	216.1731	331.4532	546.8568
Frequencies --	569.1142	916.6460	946.6604
Frequencies --	999.5722	1176.4664	1251.9747
Frequencies --	1412.3659	1459.1240	1507.2488
Frequencies --	1515.7659	3004.9856	3012.3266
Frequencies --	3056.2984	3074.9000	3100.5569

C_2H_5Br

Frequencies --	259.1178	278.2290	533.3457
Frequencies --	769.8687	965.5750	1028.8954
Frequencies --	1080.4192	1259.5398	1272.8622
Frequencies --	1414.5229	1485.0009	1489.7215
Frequencies --	1503.9311	3038.9482	3110.8288
Frequencies --	3124.0535	3146.4720	3192.8261

n-C_4H_{10} (all *anti*)

Frequencies --	118.0141	227.4386	256.9380
Frequencies --	262.7618	421.7203	733.4644
Frequencies --	808.9821	840.9937	962.1660
Frequencies --	975.7469	1019.7200	1067.6278
Frequencies --	1165.7906	1202.8930	1290.0000
Frequencies --	1318.7675	1331.5452	1397.5084
Frequencies --	1413.8111	1414.5155	1489.5184
Frequencies --	1498.6601	1507.1001	1508.1293
Frequencies --	1513.6773	1517.8134	3014.9503
Frequencies --	3021.7693	3025.7976	3027.8819
Frequencies --	3048.4671	3069.4789	3104.9901
Frequencies --	3107.7293	3108.4521	3108.8097

Mg-Br-Cl

Frequencies --	39.5004	39.5005	230.5949
Frequencies --	523.3226		

Ethene

Frequencies --	827.5783	951.7410	958.8366
Frequencies --	1056.0726	1226.2808	1363.7786
Frequencies --	1463.2025	1681.1076	3126.6268
Frequencies --	3141.7660	3212.0904	3236.9363

Ethane

Frequencies --	305.3111	819.2741	819.2747
Frequencies --	998.0355	1214.7666	1214.7683
Frequencies --	1404.3083	1423.7887	1508.0959
Frequencies --	1508.0964	1513.0878	1513.0892
Frequencies --	3036.9373	3039.8039	3106.4710
Frequencies --	3106.4712	3128.1936	3128.1951

CAT

Frequencies --	116.7418	132.3287	140.7547
Frequencies --	315.6366	354.0652	368.7725
Frequencies --	385.9175	396.3549	441.0937
Frequencies --	486.5730	496.0015	696.8103
Frequencies --	739.3579	768.7537	777.7943
Frequencies --	829.2741	877.1207	889.6425
Frequencies --	902.0786	921.9598	922.0559

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Frequencies --	1011.2075	1022.4397	1028.8311
Frequencies --	1031.5975	1227.0954	1230.0780
Frequencies --	1235.8793	1237.3890	1418.4365
Frequencies --	1420.7906	1502.7510	1502.9001
Frequencies --	1540.4548	1544.4131	3109.8422
Frequencies --	3110.0355	3110.4161	3110.5303
Frequencies --	3114.4606	3114.9368	3216.1402
Frequencies --	3216.4486	3217.4077	3218.2548

CPX

Frequencies --	3.5278	21.0812	45.3413
Frequencies --	58.6637	81.2444	93.4894
Frequencies --	116.9578	137.6768	138.7030
Frequencies --	157.0211	186.9819	212.7865
Frequencies --	244.2088	318.3636	339.0916
Frequencies --	345.9579	348.1106	402.2715
Frequencies --	409.4800	452.1998	483.3155
Frequencies --	488.7234	511.9160	529.4665
Frequencies --	741.7625	774.6661	784.0977
Frequencies --	790.7017	899.9124	905.1907
Frequencies --	922.5016	933.0333	950.3079
Frequencies --	954.5376	967.3327	991.8990
Frequencies --	1008.3119	1015.6474	1028.0812
Frequencies --	1059.9326	1067.3183	1182.0100
Frequencies --	1224.9539	1229.3959	1253.5430
Frequencies --	1260.4545	1261.8684	1408.5958
Frequencies --	1419.0502	1423.7271	1463.3519
Frequencies --	1497.9628	1505.5510	1506.8054
Frequencies --	1517.7782	1552.3471	1557.6202
Frequencies --	2970.9330	2986.8332	3010.6995
Frequencies --	3047.3279	3067.8090	3077.2639
Frequencies --	3080.1759	3121.1621	3121.4625
Frequencies --	3122.0386	3122.6211	3161.9852
Frequencies --	3173.9128	3233.9716	3235.1879

TS1

Frequencies --	**-126.6383**	46.7312	61.8495
Frequencies --	80.7705	98.3489	110.6439
Frequencies --	116.8828	128.7421	157.8007
Frequencies --	175.4912	185.0227	212.1360
Frequencies --	250.3667	266.2691	325.7790
Frequencies --	353.1340	380.2501	388.3173
Frequencies --	399.4557	413.4615	474.4708
Frequencies --	499.3980	512.2212	521.0661
Frequencies --	719.3670	755.6283	768.2046
Frequencies --	784.9408	840.1416	903.3338
Frequencies --	906.9879	911.3287	943.9593
Frequencies --	953.3284	961.5125	964.7919
Frequencies --	982.8762	986.4291	1007.3217
Frequencies --	1021.6624	1038.5457	1182.8476
Frequencies --	1216.1775	1227.8446	1240.9479
Frequencies --	1254.5038	1258.4458	1417.0166
Frequencies --	1417.8967	1419.3621	1461.3836
Frequencies --	1498.3265	1502.5663	1506.8609
Frequencies --	1520.3499	1537.2547	1547.5039
Frequencies --	2942.7694	2996.7404	3048.2381
Frequencies --	3049.6262	3079.9333	3090.3432
Frequencies --	3094.6344	3130.6993	3132.6656
Frequencies --	3134.9295	3145.0848	3179.5480
Frequencies --	3187.3760	3229.9718	3232.1137

INT1

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Frequencies --	24.9607	43.5836	74.9513
Frequencies --	80.4328	85.6459	110.4575
Frequencies --	115.2575	141.9745	160.7852
Frequencies --	197.6878	217.1639	240.9551
Frequencies --	268.9236	294.9392	327.1267
Frequencies --	340.1657	360.5941	396.0064
Frequencies --	403.9151	428.8861	442.0897
Frequencies --	457.2763	488.0196	691.5343
Frequencies --	698.6334	731.2191	740.8153
Frequencies --	771.9279	782.8010	875.7741
Frequencies --	908.0598	931.8499	941.3522
Frequencies --	968.2937	970.2209	975.4149
Frequencies --	990.1282	1013.4751	1023.9084
Frequencies --	1040.5724	1056.9503	1228.0354
Frequencies --	1236.7806	1240.4860	1249.5735
Frequencies --	1257.2660	1309.7356	1408.8349
Frequencies --	1417.8273	1422.8558	1491.1032
Frequencies --	1500.7111	1503.5067	1507.5900
Frequencies --	1510.0550	1548.1606	1555.4227
Frequencies --	2915.1870	2982.3093	3014.3276
Frequencies --	3084.9453	3088.8278	3096.7726
Frequencies --	3097.3835	3102.1982	3114.3459
Frequencies --	3116.0419	3123.4343	3193.5556
Frequencies --	3195.6644	3207.9459	3223.2263

TS2

Frequencies --	**-288.5184**	10.3243	25.3460
Frequencies --	47.5385	60.1798	69.3044
Frequencies --	74.3691	80.1076	84.6465
Frequencies --	88.2078	112.4752	125.6935
Frequencies --	131.6006	140.0019	149.6699
Frequencies --	161.5028	172.3491	180.6352
Frequencies --	199.9364	216.3386	240.4360
Frequencies --	259.4110	273.0993	291.9403
Frequencies --	320.1487	365.0874	370.2030
Frequencies --	397.6676	430.9886	465.5565
Frequencies --	501.8034	510.9302	654.9772
Frequencies --	699.9619	714.8786	737.9457
Frequencies --	760.6038	780.0607	792.6695
Frequencies --	843.5563	881.7621	908.8473
Frequencies --	923.9091	932.1389	936.2384
Frequencies --	941.5171	950.9850	990.9086
Frequencies --	997.9422	1012.0989	1020.0804
Frequencies --	1028.9700	1034.3873	1064.5782
Frequencies --	1070.7286	1180.7009	1210.0263
Frequencies --	1221.2607	1244.4685	1254.0099
Frequencies --	1259.2228	1281.0116	1397.2671
Frequencies --	1400.9278	1406.0242	1424.8145
Frequencies --	1461.4461	1477.9936	1482.4498
Frequencies --	1488.1414	1494.1776	1500.4372
Frequencies --	1504.1055	1507.7813	1561.4401
Frequencies --	1572.6505	2991.5192	3021.4749
Frequencies --	3031.2952	3059.2873	3062.5882
Frequencies --	3077.6781	3080.4498	3101.7287
Frequencies --	3107.9507	3111.8227	3113.3233
Frequencies --	3128.8170	3131.4048	3132.1872
Frequencies --	3168.3152	3186.8926	3211.6329
Frequencies --	3215.4029	3229.6096	3347.9352

INT2

Frequencies --	19.8242	31.1389	47.4975
Frequencies --	56.9510	62.9437	75.9766
Frequencies --	83.3989	88.0076	102.7167

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Frequencies --	108.0838	118.6546	150.7779
Frequencies --	161.9664	166.8703	179.1925
Frequencies --	211.1654	221.5769	224.1557
Frequencies --	235.8470	252.3563	263.4406
Frequencies --	291.9963	311.3460	340.8667
Frequencies --	362.0107	370.8753	379.6078
Frequencies --	414.0331	455.9429	481.4435
Frequencies --	501.5476	515.6650	726.3284
Frequencies --	730.9909	735.2412	754.6625
Frequencies --	759.1700	768.5507	816.0176
Frequencies --	893.2453	915.6599	928.5663
Frequencies --	936.2755	940.0339	952.2016
Frequencies --	965.9049	975.7807	983.5738
Frequencies --	1013.9203	1024.8858	1040.5874
Frequencies --	1047.9070	1052.5524	1085.4967
Frequencies --	1150.4884	1186.2637	1232.2451
Frequencies --	1242.8416	1252.0543	1259.5308
Frequencies --	1274.8250	1285.9290	1396.4113
Frequencies --	1413.3884	1416.1405	1428.9819
Frequencies --	1486.2853	1487.2736	1490.0019
Frequencies --	1493.2567	1499.6666	1500.5174
Frequencies --	1511.5642	1514.3239	1569.5846
Frequencies --	1580.5601	2930.3012	3011.4134
Frequencies --	3031.0345	3070.7348	3080.9816
Frequencies --	3088.3792	3089.6495	3100.5897
Frequencies --	3107.5159	3113.3160	3123.8584
Frequencies --	3130.1496	3133.3180	3140.9520
Frequencies --	3143.4107	3158.8880	3182.3524
Frequencies --	3188.5418	3226.4359	3238.9439

TS3

Frequencies --	**-299.3429**	16.2625	26.5245
Frequencies --	41.9050	46.0237	65.8858
Frequencies --	73.5720	85.4700	98.8708
Frequencies --	115.7697	120.6630	136.4873
Frequencies --	155.0291	176.3197	200.4296
Frequencies --	205.4217	228.3621	235.7893
Frequencies --	246.3409	277.2121	292.3476
Frequencies --	301.4090	330.6438	346.5572
Frequencies --	370.4159	377.6769	393.4184
Frequencies --	417.7783	430.5762	478.5558
Frequencies --	486.2917	494.8760	712.1956
Frequencies --	720.5307	751.0632	769.1481
Frequencies --	771.3249	780.2173	805.2294
Frequencies --	907.4049	920.1539	937.6835
Frequencies --	942.8874	958.4593	965.9444
Frequencies --	976.6269	989.5435	1009.2142
Frequencies --	1019.9639	1037.1462	1048.1534
Frequencies --	1052.4361	1068.2811	1085.1209
Frequencies --	1197.2302	1233.1099	1247.1404
Frequencies --	1253.9227	1265.7538	1270.8789
Frequencies --	1278.0796	1321.5028	1404.3332
Frequencies --	1413.6341	1418.3907	1425.2645
Frequencies --	1465.9942	1486.9623	1494.0481
Frequencies --	1500.5170	1502.4849	1505.8597
Frequencies --	1510.4233	1518.7384	1561.4591
Frequencies --	1571.1080	2861.8681	3014.9527
Frequencies --	3039.2893	3071.2391	3074.6884
Frequencies --	3102.4660	3111.3118	3112.7218
Frequencies --	3116.7813	3125.5746	3128.4998
Frequencies --	3130.0431	3134.0748	3145.1287
Frequencies --	3158.2743	3159.8854	3172.7988
Frequencies --	3191.7559	3231.3176	3233.1637

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CPL

Frequencies --	7.1474	34.7902	61.7194
Frequencies --	76.7454	93.1181	104.2298
Frequencies --	130.3394	143.1420	188.9617
Frequencies --	225.0462	240.7863	303.0786
Frequencies --	312.9952	350.7392	373.9311
Frequencies --	379.6686	422.1857	443.8594
Frequencies --	464.7912	492.1987	695.5350
Frequencies --	736.7250	756.9923	775.5542
Frequencies --	792.1731	903.9469	920.7003
Frequencies --	927.8212	958.5191	975.3408
Frequencies --	1004.8980	1012.3073	1042.8250
Frequencies --	1063.6551	1219.1481	1247.0821
Frequencies --	1256.8975	1258.5174	1413.0854
Frequencies --	1421.4448	1491.5102	1509.8799
Frequencies --	1554.9189	1559.8558	3063.7191
Frequencies --	3094.1817	3097.9164	3104.7366
Frequencies --	3123.1592	3126.1890	3166.2913
Frequencies --	3195.3126	3213.2715	3231.2958

TS β-H (1)

Frequencies --	**-1006.9712**	-8.2807	33.8232
Frequencies --	38.0367	44.6596	61.6239
Frequencies --	86.5533	95.1392	103.2098
Frequencies --	110.1975	116.1332	138.9981
Frequencies --	151.8802	165.1273	184.0440
Frequencies --	196.9769	207.2839	225.9438
Frequencies --	250.3931	259.6015	278.4197
Frequencies --	287.8594	300.4647	336.4408
Frequencies --	362.7269	379.5574	395.3265
Frequencies --	419.5056	426.5941	448.4243
Frequencies --	481.9056	493.7768	513.0475
Frequencies --	677.9276	701.4281	749.3716
Frequencies --	769.4289	771.8129	791.6532
Frequencies --	801.4822	857.3526	906.9864
Frequencies --	925.9283	940.8334	965.6396
Frequencies --	972.7835	976.4626	987.8226
Frequencies --	990.0596	1022.0900	1032.9608
Frequencies --	1040.1580	1045.7327	1090.3165
Frequencies --	1109.1188	1117.5512	1211.5685
Frequencies --	1243.0029	1247.5329	1255.2410
Frequencies --	1257.7797	1262.9663	1285.7275
Frequencies --	1304.9138	1412.2760	1413.5690
Frequencies --	1431.3826	1456.1267	1480.5632
Frequencies --	1492.3448	1501.4868	1510.8175
Frequencies --	1519.6855	1535.7160	1562.2013
Frequencies --	1570.9871	1963.7658	3011.9106
Frequencies --	3045.3098	3058.9055	3081.0903
Frequencies --	3086.6502	3098.6896	3105.5866
Frequencies --	3107.8026	3129.4096	3142.7077
Frequencies --	3149.0733	3163.9131	3168.6023
Frequencies --	3177.4926	3183.6727	3193.9387
Frequencies --	3243.1328	3250.6227	3263.2020

TS β-H (2)

Frequencies --	**-1020.7765**	26.7303	34.9159
Frequencies --	53.7331	66.7764	77.3741
Frequencies --	96.6566	113.5430	121.2798
Frequencies --	125.8424	133.6221	140.6226
Frequencies --	170.2007	177.8362	184.2869
Frequencies --	199.7014	209.3169	238.5102

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Frequencies --	246.1884	264.4811	273.6459
Frequencies --	291.0144	312.2003	327.4603
Frequencies --	359.3493	395.2853	397.5160
Frequencies --	409.0461	442.9938	486.1623
Frequencies --	500.9187	519.4791	575.7833
Frequencies --	732.8189	756.3236	772.6860
Frequencies --	776.4721	783.5792	825.2689
Frequencies --	845.8606	848.6093	913.1614
Frequencies --	922.7560	936.7040	939.4476
Frequencies --	961.8670	969.7254	975.7120
Frequencies --	1023.5005	1024.5174	1036.8426
Frequencies --	1040.7618	1045.5849	1088.8920
Frequencies --	1114.6887	1124.0561	1130.5899
Frequencies --	1219.5113	1232.5079	1236.8189
Frequencies --	1253.0999	1264.5332	1268.4363
Frequencies --	1304.1327	1422.0584	1424.2147
Frequencies --	1432.9962	1459.2515	1490.4962
Frequencies --	1502.5629	1512.2445	1518.8942
Frequencies --	1524.0718	1535.0489	1564.2793
Frequencies --	1597.5203	1948.1551	2994.8387
Frequencies --	3028.5784	3067.2541	3080.3985
Frequencies --	3085.8701	3098.0568	3099.5098
Frequencies --	3122.8826	3127.2771	3137.6627
Frequencies --	3149.2364	3152.2269	3157.3092
Frequencies --	3158.4931	3189.0149	3192.8706
Frequencies --	3238.6658	3252.4583	3258.8915

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5. Cartesian Coordinates of Optimised Structures

C_2H_5MgCl

12	0.000000	0.295038	0.000000
17	-2.143585	1.034584	0.000000
6	1.970917	-0.411838	0.000000
1	2.469973	0.028762	0.875415
1	2.469973	0.028762	-0.875415
6	2.168376	-1.943764	0.000000
1	3.232884	-2.221064	0.000000
1	1.716175	-2.415615	0.880911
1	1.716175	-2.415615	-0.880911

C_2H_5Br

6	1.049381	0.691132	0.000001
1	1.086932	1.316178	-0.892533
1	1.086961	1.316173	0.892540
6	2.098468	-0.404907	0.000002
1	3.091891	0.063101	-0.000173
1	2.020711	-1.037455	0.889062
1	2.020496	-1.037627	-0.888921
35	-0.805545	-0.066792	0.000000

n-C_4H_{10} (all *anti*)

6	0.009317	-0.016137	0.026639
1	0.016531	-0.028632	1.123111
1	1.051808	-0.051610	-0.313797
1	-0.481208	-0.936697	-0.313797
6	-0.708623	1.227370	-0.516151
1	-1.737795	1.252513	-0.130679
1	-0.215811	2.131231	-0.130679
6	-0.743303	1.287439	-2.050515
1	-1.236115	0.383578	-2.435988
1	0.285869	1.262296	-2.435988
6	-1.461242	2.530946	-2.593306
1	-0.970718	3.451507	-2.252870
1	-1.468457	2.543442	-3.689777
1	-2.503734	2.566420	-2.252870

Mg-Br-Cl

17	0.000000	0.000000	-2.925696
35	0.000000	0.000000	1.660003
12	0.000000	0.000000	-0.696938

Ethene

1	0.000000	0.927933	1.240620
6	0.000000	0.000000	0.669050
6	0.000000	0.000000	-0.669050
1	0.000000	-0.927933	-1.240620
1	0.000000	-0.927933	1.240620
1	0.000000	0.927933	-1.240620

Ethane

1	0.000000	1.021347	1.165082
6	0.000000	0.000000	0.767832
6	0.000000	0.000000	-0.767832
1	0.000000	-1.021347	-1.165082
1	-0.884512	-0.510673	1.165082
1	-0.884512	0.510673	-1.165082
1	0.884512	-0.510673	1.165082
1	0.884512	0.510673	-1.165082

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CAT

6	2.864573	-1.880280	0.191592
6	1.716450	-1.778039	-0.630341
1	0.773494	-2.195655	-0.292871
6	3.062531	1.869476	0.557804
1	2.993087	1.789284	1.644388
6	1.886647	1.951637	-0.228532
1	1.972579	2.318743	-1.254703
6	0.731455	1.211660	0.121651
1	0.476282	1.056334	1.171818
1	3.988346	2.297522	0.180908
1	-0.098540	1.142106	-0.576628
1	1.819614	-1.668289	-1.711635
28	2.389841	0.039423	-0.014878
6	4.037525	-1.146181	-0.112938
1	4.841540	-1.097915	0.617715
1	4.341521	-0.999134	-1.151130
1	2.739239	-2.258394	1.209738

CPX

6	1.820652	1.319353	1.292897
6	0.476101	0.923766	1.577119
1	-0.265701	1.727488	1.551141
6	2.589179	-0.973703	-1.359416
1	2.658501	-0.118821	-2.034177
6	1.394052	-1.693075	-1.226615
1	1.414883	-2.668759	-0.735236
6	0.138981	-1.031314	-1.394072
1	0.047875	-0.271388	-2.173836
1	3.530645	-1.432544	-1.069848
1	-0.750842	-1.651513	-1.259932
1	0.307028	0.182180	2.362054
28	1.319289	-0.150278	0.038367
6	2.852466	0.372325	1.313259
1	3.837131	0.638893	0.939050
1	2.808225	-0.493062	1.976586
1	1.994510	2.281556	0.805344
12	-1.454077	0.203177	0.150710
17	-1.948573	2.050442	-1.191446
6	-2.691338	-1.100504	1.270887
1	-3.034079	-0.564755	2.172318
1	-2.071497	-1.927390	1.657887
6	-3.925652	-1.691422	0.548822
1	-3.637752	-2.303429	-0.317462
1	-4.543468	-2.335253	1.195743
1	-4.587527	-0.903616	0.164876

TS1

6	-1.489513	-1.950442	0.300199
6	-0.100082	-2.173413	0.102625
1	0.203931	-2.796790	-0.738303
6	-2.640330	0.614333	-1.123074
1	-2.742077	-0.198104	-1.841500
6	-1.553130	1.500165	-1.202617
1	-1.600271	2.467854	-0.701776
6	-0.301774	0.998492	-1.668442
1	-0.302222	0.258347	-2.470239
1	-3.552852	0.920968	-0.617292
1	0.545292	1.687265	-1.680009
1	0.506570	-2.301545	1.008333
28	-1.017094	0.017105	0.016605
6	-2.005437	-1.171693	1.366490

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1	-3.082623	-1.053838	1.454453
1	-1.444420	-1.085101	2.295533
1	-2.174274	-2.276356	-0.484798
12	1.373019	-0.280141	0.022142
17	3.553480	-0.541311	-0.571665
6	0.435945	0.970847	1.577934
1	0.976766	0.399449	2.357630
1	-0.542119	1.146685	2.038705
6	1.130569	2.341197	1.379331
1	0.582268	2.968525	0.665366
1	1.204961	2.915560	2.314693
1	2.156815	2.255202	0.992184

INT1

6	0.194204	2.272095	-0.508037
6	-1.157707	2.491158	-0.175628
1	-1.825370	2.866171	-0.950424
6	2.268330	-0.244835	-1.661335
1	1.638488	0.166544	-2.450788
6	1.963621	-1.490344	-1.087038
1	2.727977	-1.996167	-0.491611
6	0.609205	-1.876798	-0.926889
1	-0.103818	-1.656635	-1.725480
1	3.286311	0.135897	-1.620854
1	0.371579	-2.758556	-0.335385
1	-1.409735	2.779931	0.848684
28	0.995220	-0.083722	-0.020015
6	1.273583	1.925633	0.353503
1	2.273064	2.144054	-0.020462
1	1.139221	2.124613	1.418169
1	0.427297	2.291081	-1.578047
12	-1.484792	0.289039	0.029513
17	-3.417712	-0.855605	-0.376898
6	-0.094372	-0.408841	1.656943
1	-0.565577	0.474275	2.135059
1	-0.841648	-1.221503	1.702130
6	1.076158	-0.843006	2.562120
1	1.860543	-0.079136	2.610444
1	0.740747	-1.030893	3.592073
1	1.535257	-1.769003	2.198195

TS2

6	0.081625	-2.057440	-1.259847
6	-1.227337	-1.731895	-1.753095
1	-1.859781	-2.622429	-1.867445
6	1.495904	-1.819478	1.761763
1	0.571939	-1.355624	2.106844
6	2.719288	-1.169148	1.911432
1	3.635549	-1.745333	1.757706
6	2.800852	0.254905	1.894040
1	2.012507	0.833036	2.378380
1	1.463399	-2.894922	1.606075
1	3.780816	0.727293	1.904948
1	-1.233493	-1.108760	-2.655008
28	2.055071	-0.389814	0.151283
6	1.289530	-1.429833	-1.553861
1	2.190573	-2.033933	-1.407880
1	1.317385	-0.744651	-2.400275
1	0.131302	-2.911110	-0.578209
12	-2.602463	-0.743478	-0.410564
17	-4.335900	-1.663818	0.755551
6	3.034092	0.912769	-0.935473
1	2.468139	1.173896	-1.840381

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1	3.231061	1.845261	-0.394383
6	4.365115	0.248163	-1.321439
1	4.217933	-0.685218	-1.879203
1	4.975521	0.905970	-1.961106
1	4.971808	0.007533	-0.439383
35	-2.253724	1.765733	-0.098277
6	0.118397	1.485847	0.131154
1	0.010704	0.822619	0.980222
1	0.204718	1.037119	-0.846838
6	0.632171	2.873377	0.371207
1	0.762056	3.423925	-0.562495
1	-0.033621	3.434925	1.033329
1	1.601870	2.807594	0.876002

INT2

6	0.174832	1.068294	2.120083
6	-1.137257	0.695678	2.363343
1	-1.852853	1.468571	2.658705
6	2.491391	2.033578	-0.228538
1	1.496342	2.308354	-0.581906
6	3.307043	1.196109	-0.984204
1	4.349403	1.078268	-0.682393
6	2.731442	0.235974	-1.854426
1	1.829151	0.493553	-2.409319
1	2.904254	2.636362	0.576154
1	3.369097	-0.508271	-2.325813
1	-1.370815	-0.323435	2.676872
28	1.910711	-0.088620	0.019290
6	1.313825	0.202699	1.974560
1	2.232137	0.667832	2.344495
1	1.165464	-0.804598	2.370614
1	0.360879	2.140162	2.001396
12	-1.988022	0.686631	0.262452
17	-1.483515	2.504039	-1.050234
6	2.630388	-1.896830	0.196173
1	1.973257	-2.462058	0.860385
1	2.703061	-2.394714	-0.769680
6	3.993623	-1.630609	0.819451
1	3.942021	-0.994162	1.709655
1	4.420724	-2.591504	1.146544
1	4.700370	-1.185098	0.113403
35	-3.789953	-0.908678	-0.102007
6	0.294550	-1.021109	-0.512877
1	-0.101782	-0.076251	-0.934710
1	-0.230016	-1.301332	0.407913
6	0.186630	-2.123814	-1.553781
1	0.575218	-3.076883	-1.183451
1	-0.871529	-2.285362	-1.802513
1	0.711291	-1.872378	-2.480368

TS3

6	0.241076	1.056940	2.163402
6	-1.099845	0.726757	2.346369
1	-1.772569	1.515616	2.697638
6	2.477749	1.983470	-0.038790
1	1.532710	2.423369	-0.356891
6	3.243674	1.231778	-0.953758
1	4.295010	1.033036	-0.736133
6	2.578843	0.443946	-1.905254
1	1.631504	0.778786	-2.326467
1	2.963221	2.455590	0.812001
1	3.134737	-0.281005	-2.495751
1	-1.367238	-0.290260	2.641337

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28	1.925318	0.001963	0.045034
6	1.350261	0.163344	2.019947
1	2.279986	0.571366	2.424491
1	1.153048	-0.856334	2.360209
1	0.468016	2.125465	2.096389
12	-2.003310	0.788464	0.299058
17	-1.308176	2.361831	-1.217497
6	2.415497	-2.020246	-0.005125
1	1.869736	-2.863640	0.417372
1	2.705664	-2.265693	-1.025312
6	3.658500	-1.788753	0.876370
1	3.409999	-1.618823	1.925703
1	4.247435	-2.717619	0.826394
1	4.311951	-0.981216	0.535519
35	-3.795953	-0.816343	-0.074599
6	0.502198	-1.355302	-0.413818
1	0.091469	-0.344716	-0.634829
1	0.010696	-1.755089	0.474671
6	0.256290	-2.223838	-1.640755
1	0.564970	-3.262093	-1.484903
1	-0.819155	-2.233178	-1.858995
1	0.771488	-1.837790	-2.525225

CPL

6	0.764585	2.222261	-0.357058
6	-0.593626	2.434381	-0.017799
1	-1.224727	2.890124	-0.783000
6	3.383596	0.030522	-1.262872
1	2.824201	0.076693	-2.200265
6	3.498807	-1.205905	-0.571383
1	4.294879	-1.341507	0.164188
6	2.384036	-2.049927	-0.545348
1	1.694301	-2.092450	-1.389529
1	4.168000	0.776344	-1.153118
1	2.338803	-2.881832	0.153202
1	-0.795227	2.781291	1.001916
28	1.949077	-0.113361	0.100736
6	1.838072	1.902317	0.505187
1	2.823116	2.232603	0.178568
1	1.661689	1.998300	1.579200
1	1.009062	2.277628	-1.423402
12	-1.443926	0.442607	0.257454
17	0.163270	-0.817323	1.436978
35	-3.613416	-0.427480	-0.370594

TS β-H (1)

6	0.155354	0.926390	1.950615
6	-1.130071	0.498820	2.268627
1	-1.810196	1.248403	2.690688
6	1.206532	1.413889	-1.080768
1	0.377606	1.063573	-1.688778
6	2.536111	1.159424	-1.485525
1	3.334494	1.789274	-1.098448
6	2.846494	-0.063314	-2.098199
1	2.111543	-0.576625	-2.714694
1	0.999463	2.290886	-0.475384
1	3.885197	-0.344418	-2.254714
1	-1.294798	-0.527385	2.602587
28	2.000635	-0.291476	-0.151617
6	1.342543	0.137567	1.793443
1	2.227256	0.691730	2.108991
1	1.282853	-0.853252	2.251356
1	0.278328	2.006283	1.820050

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12	-2.353321	0.697241	0.396432
17	-2.369403	2.748096	-0.615523
6	3.895711	-0.802475	0.721694
1	3.696468	-1.198763	1.722261
1	4.450960	-1.566484	0.164539
6	4.754982	0.462769	0.812221
1	4.237831	1.294631	1.302346
1	5.660874	0.251505	1.400143
1	5.091840	0.806588	-0.170942
35	-3.753714	-1.201393	-0.193248
6	0.338704	-1.507981	-0.685478
1	0.092693	-1.342530	-1.731008
1	-0.464055	-1.344416	0.027343
6	1.384611	-2.391488	-0.334406
1	2.553262	-1.690303	0.111533
1	1.296220	-2.937087	0.607079
1	1.888262	-2.937658	-1.132608

TS β-H (2)

6	0.238297	0.917311	2.096475
6	-1.047101	0.492035	2.328708
1	-1.812771	1.225176	2.597911
6	2.350923	1.845913	-0.133772
1	1.391776	2.166042	-0.536903
6	3.290243	1.184154	-0.964824
1	4.337201	1.162165	-0.664561
6	2.832393	0.303985	-1.949443
1	1.884190	0.479663	-2.447574
1	2.713066	2.414086	0.719651
1	3.530122	-0.357506	-2.459021
1	-1.258037	-0.549611	2.575905
28	2.126849	-0.185100	0.058446
6	1.428444	0.092130	1.970116
1	2.283987	0.575590	2.445959
1	1.283438	-0.925442	2.345844
1	0.384854	1.996805	2.000937
12	-1.893032	0.569822	0.169618
17	-1.662300	2.635345	-0.823199
6	2.859637	-2.196631	0.294327
1	2.326734	-2.814961	1.019475
1	3.135925	-2.717809	-0.622673
6	3.768928	-1.223379	0.804990
1	3.848920	-1.072961	1.877405
1	4.654878	-0.976211	0.226211
35	-3.813852	-0.918306	-0.057415
6	0.207419	-0.789658	-0.711638
1	-0.024845	0.251825	-0.978381
1	-0.354706	-1.134804	0.166471
6	-0.049823	-1.713981	-1.908754
1	1.659210	-1.630199	-0.226320
1	0.556287	-1.429457	-2.774570
1	0.193668	-2.755198	-1.667939
1	-1.101534	-1.693691	-2.222964