

Supplementary information

2-mtea conformer 1 XIAM assigned lines

J'	Ka'	Kc'	J''	Ka''	Kc''	F''	F''	Vcalc/MHz	Vobs/MHz	Vobs-calc/MHz	state
3	2	2	3	1	2	3	3	13469.7115	13469.713	0.0015	/A
						4	4	13469.9513	13469.9505	-0.0008	/A
						2	2	13470.0349	13470.0374	0.0025	/A
						3	3	13468.7945	13468.7931	-0.0014	/E
						4	4	13469.0316	13469.0287	-0.0029	/E
						2	2	13469.1142	13469.1125	-0.0017	/E
3	2	1	3	1	3	2	2	13842.8158	13842.818	0.0022	/A
						4	4	13843.0599	13843.0585	-0.0014	/A
						3	3	13843.7586	13843.7614	0.0028	/A
						2	2	13843.5661	13843.5657	-0.0005	/E
						4	4	13843.8093	13843.8066	-0.0027	/E
						3	3	13844.5053	13844.505	-0.0002	/E
2	1	1	1	0	1	1	0	13459.1323	13459.1378	0.0054	/E
						3	2	13459.6949	13459.6966	0.0017	/E
						2	1	13460.2628	13460.2638	0.001	/E
						1	0	13459.1997	13459.1956	-0.0041	/A
						3	2	13459.7622	13459.7625	0.0003	/A
						2	1	13460.3301	13460.3261	-0.0041	/A

3	0	3	2	0	2	4	3	13220.8838	13220.887	0.0032	/E
						4	3	13220.921	13220.9204	-0.0006	/A
2	0	2	1	0	1	3	2	8815.0552	8815.0513	-0.0039	/E
						3	2	8815.0804	8815.0788	-0.0016	/A
1	1	0	0	0	0	2	1	8990.1935	8990.1975	0.0039	/E
						1	1	8990.7425	8990.7442	0.0016	/E
						2	1	8990.2264	8990.2254	-0.0009	/A
						1	1	8990.7755	8990.7736	-0.0019	/A
3	0	3	2	1	1	3	2	8575.6315	8575.6304	-0.0011	/E
						4	3	8576.2442	8576.2417	-0.0024	/E
						3	2	8575.6265	8575.6304	0.0039	/A
						4	3	8576.2392	8576.2417	0.0026	/A
4	2	3	4	1	3	4	4	13347.2284	13347.2199	-0.0085	/A
						5	5	13347.5618	13347.5599	-0.0019	/A
						3	3	13347.6474	13347.6564	0.009	/A
						4	4	13346.8497	13346.853	0.0034	/E
						5	5	13347.1821	13347.185	0.0029	/E
						3	3	13347.2674	13347.2665	-0.0009	/E
5	2	4	5	1	4	5	5	13194.6002	13194.6045	0.0043	/A
						6	6	13194.9826	13194.9798	-0.0028	/A
						4	4	13195.0604	13195.0575	-0.0029	/A

[illegible]

[illegible]

[illegible]

3	1	3	2	0	2	3	2	17745.1317	17745.1289	-0.0027	/A
						4	3	17745.7902	17745.7978	0.0077	/A
						2	1	17746.0784	17746.072	-0.0064	/A
						3	2	17745.0984	17745.0981	-0.0003	/E
								0			
						4	3	17745.757	17745.759	0.002	/E
						2	1	17746.0452	17746.044	-0.0012	/E
8	2	6	8	1	7	8	8	12916.557	12916.5572	0.0003	/A
						8	8	12916.6628	12916.6638	0.001	/E
3	2	2	3	1	2	3	3	13698.15	13698.1463	-0.0037	/E
						4	4	13698.9695	13698.9698	0.0002	/E
						2	2	13699.2557	13699.2572	0.0015	/E
3	2	1	3	1	3	2	2	14074.114	14074.118	0.004	/E
						4	4	14074.2501	14074.2446	-0.0055	/E
						3	3	14074.641	14074.6396	-0.0014	/E
4	2	3	4	1	4	3	3	14194.7294	14194.7423	0.0129	/A
						5	5	14194.8519	14194.8513	-0.0006	/A
						4	4	14195.3294	14195.3382	0.0088	/A
						3	3	14194.1961	14194.1997	0.0036	/E
						5	5	14194.3189	14194.3131	-0.0058	/E
						4	4	14194.7979	14194.7965	-0.0014	/E

APS conformer 1 SPFIT assigned lines

J'	Ka'	Kc'	J''	Ka''	Kc''	Vobs/MHz	Vobs-calc/MHz
5	1	5	4	1	4	7544.9697	0.0002
5	0	5	4	0	4	7691.6042	0.0001
5	0	5	4	1	4	7060.4044	-0.0003
5	1	5	4	0	4	8176.1649	-0.0037
6	0	6	5	1	5	8685.2549	-0.0002
6	1	6	5	0	5	9522.745	0.0001
6	1	6	5	1	5	9038.1794	-0.0007
6	0	6	5	0	5	9169.8199	0.0001
5	1	4	4	0	4	9701.626	0.0006
6	1	5	5	1	4	9633.5031	-0.0001
6	1	5	5	0	5	11643.524	-0.0006
7	0	7	6	0	6	10632.6736	0
7	1	7	6	0	6	10878.1298	0.0004
7	0	7	6	1	6	10279.7487	0
7	1	7	6	1	6	10525.2048	0.0004
8	0	8	7	0	7	12087.691	0.0001
8	1	8	7	1	7	12006.5742	0.0008
8	0	8	7	1	7	11842.235	-0.0002
8	1	8	7	0	7	12252.0293	0.0003
6	1	5	5	2	4	7210.1773	-0.0029
5	2	4	4	1	3	10472.8447	0.001
5	1	4	4	1	3	8049.5205	-0.0001
7	1	6	6	2	5	9048.2381	0.0008
7	1	6	6	1	5	11200.5028	0.0003
6	2	5	5	2	4	9362.4452	-0.0003
7	3	5	6	2	4	15919.4799	-0.0006
8	2	6	7	3	5	8186.3389	0.0001
8	2	6	7	2	5	12873.8647	0.0004
7	2	5	6	2	4	11231.9552	0.0001
8	3	6	7	3	5	12579.4544	-0.0001
8	4	5	7	4	4	12577.9734	0
7	4	4	7	3	5	7332.8154	0.0005
8	4	5	8	3	6	7331.3335	-0.0002
5	2	3	4	2	2	7951.7509	0.0003
6	2	4	5	2	3	9588.1544	-0.0005
6	3	4	5	3	3	9427.9093	0.0001
7	3	5	6	3	4	11004.1722	-0.0007

5	3	3	4	2	2	13027.3039	0
6	2	4	5	1	5	13784.5402	0.001
5	2	3	4	1	4	11741.3534	-0.0003
4	3	1	3	2	2	11545.0179	0
4	3	2	3	2	1	11505.6338	-0.0002
4	3	2	3	2	2	11542.6413	-0.0001
4	3	1	3	2	1	11508.0108	0.0001
4	2	2	3	1	2	9221.4356	-0.0004
4	2	3	3	1	3	9725.8102	0.0006
4	2	3	3	1	2	9112.1764	0.0004
4	2	2	3	1	3	9835.0702	0.0005
4	4	0	4	3	1	7349.3367	0.002
4	4	1	4	3	2	7351.6979	-0.0005
3	2	1	2	1	1	7737.6914	0.0011
3	2	2	2	1	2	8007.6698	-0.002
3	2	2	2	1	1	7700.6833	0.0003
3	2	1	2	1	2	8044.6804	0.0012
3	3	1	2	2	0	9955.3192	0.0001
3	3	0	2	2	1	9963.1127	-0.0002
3	3	0	2	2	0	9955.6597	0
3	3	1	2	2	1	9962.7721	-0.0003
4	2	2	3	1	2	9221.4356	-0.0004
4	2	3	3	1	3	9725.8102	0.0006
4	2	3	3	1	2	9112.1764	0.0004
4	2	2	3	1	3	9835.0702	0.0005
4	1	4	3	0	3	6823.0143	0.0007
4	1	3	3	0	3	7843.9199	0.0009
6	2	4	5	1	4	12259.0824	0
6	2	5	5	1	5	13311.2248	-0.0003
6	2	5	5	1	4	11785.7687	0.0001
5	2	3	4	1	3	10720.447	-0.0012
5	2	4	4	1	4	11493.7489	-0.0001
5	3	2	4	2	2	13036.7549	0.0003
5	3	3	4	2	3	13136.5656	0.0016
7	3	5	6	2	5	16392.7939	-0.0006
7	1	6	6	2	4	8574.9246	0.0014
5	3	3	4	3	2	7852.1376	-0.0002
7	2	6	6	2	5	10904.2662	0
5	4	2	5	3	3	7345.9448	0.0014
5	4	1	4	3	2	15198.1973	0
6	3	3	5	2	3	14531.5235	0.0005
6	3	4	5	2	4	14751.0659	-0.0011

7	3	4	6	3	3	11045.0932	0.001
7	2	6	6	2	5	10904.2662	0
5	5	0	5	4	1	9452.983	-0.0019
5	5	1	5	4	2	9453.0967	-0.0037
7	0	7	6	1	5	8158.9698	0.0009
7	2	6	6	1	6	15177.3106	-0.0006
8	1	7	7	1	6	12746.1231	0.0002
8	2	7	7	2	6	12437.9706	0.0003
6	4	2	6	3	3	7311.4492	-0.0026
6	4	2	5	3	3	16767.4217	0.0003
7	4	4	7	3	4	7263.8346	-0.0006
7	4	3	7	3	5	7334.9212	-0.0003
8	3	5	7	3	4	12658.3459	0.0001
8	4	4	7	4	3	12582.134	-0.0007
6	5	1	6	4	2	9445.8844	0.0019
8	5	4	8	4	5	9421.9793	0.0015
8	0	8	7	1	6	9046.1558	-0.0014
8	1	7	7	2	5	10089.0923	0.0012
8	5	3	8	4	4	9415.836	0.0006
7	4	3	7	3	4	7265.9414	-0.0004
7	5	3	7	4	4	9436.2994	0.0013
8	1	7	7	0	7	15787.6546	-0.0018
8	2	6	7	3	4	8117.3604	0.0012
8	4	4	8	3	6	7337.602	0.0002
5	2	4	4	2	3	7813.4055	-0.0004
5	3	2	4	3	1	7859.2119	0
6	4	3	5	4	2	9420.8997	-0.0005
5	3	2	4	2	3	13146.0151	0.0004
5	4	2	4	3	1	15195.705	0.0003
6	4	3	5	3	2	16757.3932	0.0002
7	2	5	6	1	6	15978.3145	0.0003
6	4	3	6	3	3	7310.874	0
6	4	2	6	3	4	7339.5124	0.0001
8	4	5	8	3	5	7183.4625	-0.0003
5	4	1	5	3	2	7336.6094	0.0007
8	2	6	7	1	6	15530.8952	-0.0009

All geometries were calculated using Density Functional theory at the B3LYP(D3)-BJ level of theory with aug-cc-pVTZ basis set.

APS conformer 1

1	16	1.244848	1.366518	0.402734
2	6	-0.357873	0.608898	0.190960
3	6	-1.078897	0.811762	-0.985132
4	6	-2.324077	0.220031	-1.150645
5	6	-2.862416	-0.567482	-0.138354
6	6	-2.149406	-0.764934	1.037447
7	6	-0.897557	-0.183436	1.201205
8	6	2.278193	0.186539	-0.585429
9	6	2.326078	-1.162851	0.035938
10	6	1.698498	-2.226348	-0.450910
11	1	-2.563356	-1.377385	1.826692
12	1	-0.331880	-0.342860	2.107307
13	1	-0.662538	1.437549	-1.762069
14	1	-2.877924	0.381029	-2.065423
15	1	-3.834829	-1.022786	-0.265777
16	1	1.883129	0.152811	-1.598753
17	1	3.259262	0.660506	-0.609243
18	1	2.876618	-1.238113	0.967133
19	1	1.121039	-2.170799	-1.365215
20	1	1.734858	-3.184055	0.049385

APS conformer 2

1	16	-1.045760	-1.321620	-0.028771
2	6	0.490010	-0.429937	-0.049213
3	6	0.627071	0.901157	-0.438412
4	6	1.880413	1.503423	-0.422383
5	6	3.002630	0.797686	-0.011401
6	6	2.863533	-0.528851	0.385219
7	6	1.620475	-1.141063	0.364684
8	6	-2.218674	-0.208747	-0.863037
9	6	-2.792335	0.924954	-0.063213
10	6	-2.510054	1.234592	1.192655
11	1	3.728288	-1.093076	0.706832
12	1	1.522002	-2.176165	0.663295
13	1	-0.233291	1.479888	-0.733871

14	1	1.971853	2.537119	-0.727428
15	1	3.973087	1.273099	0.002143
16	1	-1.749655	0.162834	-1.776503
17	1	-3.023028	-0.872116	-1.187759
18	1	-3.510305	1.527739	-0.612561
19	1	-1.799635	0.658253	1.769738
20	1	-2.984588	2.075175	1.678878

APS conformer 3

1	16	-0.913585	1.330932	-0.255770
2	6	0.600975	0.414784	-0.109145
3	6	1.655100	1.063777	0.540891
4	6	2.888595	0.444711	0.667413
5	6	3.090891	-0.835303	0.161019
6	6	2.043395	-1.483958	-0.478229
7	6	0.805651	-0.866563	-0.619158
8	6	-2.150325	0.069152	-0.748682
9	6	-2.495605	-0.880099	0.349527
10	6	-3.710763	-1.005513	0.866494
11	1	2.184407	-2.479715	-0.876304
12	1	0.013881	-1.392950	-1.129059
13	1	1.501566	2.053490	0.949353
14	1	3.693199	0.962284	1.171667
15	1	4.050975	-1.319932	0.267033
16	1	-3.018882	0.655219	-1.045324
17	1	-1.783281	-0.441883	-1.638381
18	1	-1.681684	-1.482122	0.736118
19	1	-4.543693	-0.411975	0.509471
20	1	-3.914898	-1.703413	1.666583

APS conformer 4

1	16	-0.924452	0.882649	-0.140588
2	6	0.735743	0.261234	-0.051045
3	6	1.756907	1.212820	0.032309
4	6	3.083480	0.814303	0.072651
5	6	3.415714	-0.536752	0.041494
6	6	2.403099	-1.482434	-0.037737
7	6	1.069218	-1.092314	-0.089998
8	6	-1.951623	-0.605371	0.181816
9	6	-3.344490	-0.163479	0.485361
10	6	-4.384909	-0.391711	-0.304825
11	1	2.646297	-2.535986	-0.065740
12	1	0.303160	-1.847962	-0.168824
13	1	1.505608	2.264167	0.071105
14	1	3.861269	1.562915	0.137470
15	1	4.450578	-0.845861	0.079482
16	1	-1.930855	-1.262739	-0.685499
17	1	-1.514663	-1.122800	1.035984
18	1	-3.476716	0.386932	1.410125
19	1	-4.277953	-0.925938	-1.240819
20	1	-5.377923	-0.054111	-0.042864

APS conformer 5

1	16	-0.950628	-0.481863	0.820405
2	6	0.731373	-0.172405	0.300881
3	6	1.274055	1.111253	0.362123
4	6	2.587973	1.332448	-0.026928
5	6	3.377066	0.271715	-0.460102
6	6	2.844010	-1.010058	-0.508328
7	6	1.522790	-1.232369	-0.136373
8	6	-1.880694	0.357393	-0.543703
9	6	-3.299818	0.539182	-0.128871
10	6	-4.324545	-0.098289	-0.680211
11	1	3.452852	-1.838775	-0.842901
12	1	1.098596	-2.225055	-0.184472
13	1	0.668120	1.929848	0.724923
14	1	3.000631	2.330912	0.021048
15	1	4.402858	0.444466	-0.754732
16	1	-1.395331	1.317446	-0.713018

17	1	-1.801605	-0.246125	-1.445728
18	1	-3.470416	1.229470	0.690103
19	1	-4.181471	-0.805132	-1.488261
20	1	-5.339304	0.065426	-0.344938

APS conformer 6

1	16	-1.017616	-0.710649	-0.001811
2	6	0.685061	-0.214898	-0.000560
3	6	1.133246	1.105463	-0.001032
4	6	2.497783	1.377666	-0.000225
5	6	3.427493	0.348337	0.000943
6	6	2.980295	-0.970006	0.001367
7	6	1.624418	-1.251874	0.000687
8	6	-1.901357	0.881801	0.000246
9	6	-3.389831	0.721336	0.001305
10	6	-4.080710	-0.409551	0.001397
11	1	3.691796	-1.784452	0.002322
12	1	1.285521	-2.279232	0.001191
13	1	0.436600	1.928460	-0.002083
14	1	2.829018	2.407342	-0.000567
15	1	4.485874	0.566651	0.001542
16	1	-1.596798	1.452196	0.880274
17	1	-1.598391	1.453782	-0.879299
18	1	-3.925026	1.665848	0.002015
19	1	-3.603835	-1.380154	0.000735
20	1	-5.161535	-0.397240	0.002182

APS conformer 7

1	16	-1.045387	-0.334804	0.715988
2	6	0.678945	-0.127291	0.291328
3	6	1.289354	1.120905	0.407738
4	6	2.632510	1.272448	0.088978

5	6	3.377647	0.177304	-0.334688
6	6	2.774571	-1.069906	-0.441047
7	6	1.427788	-1.223098	-0.132273
8	6	-1.790379	0.330717	-0.825889
9	6	-3.284917	0.335990	-0.811753
10	6	-4.078323	-0.068406	0.170084
11	1	3.350617	-1.925242	-0.766584
12	1	0.951136	-2.189254	-0.216395
13	1	0.710392	1.964944	0.755408
14	1	3.099499	2.243529	0.180566
15	1	4.424801	0.295555	-0.576510
16	1	-1.416494	1.345613	-0.973050
17	1	-1.427184	-0.269679	-1.662178
18	1	-3.729201	0.720689	-1.725051
19	1	-3.690553	-0.460450	1.100677
20	1	-5.153657	-0.018622	0.071580

2-mtea conformer 1

1	6	-1.794572	1.046332	-0.086150
2	16	-1.025210	-0.595512	-0.243004
3	1	-2.098430	1.229813	0.943298
4	1	-2.677989	1.039749	-0.720416
5	1	-1.127829	1.837049	-0.422592
6	6	0.352230	-0.424755	0.945696

7	6	1.479684	0.500639	0.479003
8	1	0.729605	-1.439145	1.082232
9	1	-0.054646	-0.091330	1.902673
10	7	2.150854	0.119624	-0.756399
11	1	2.228302	0.556246	1.273248
12	1	1.090988	1.513499	0.357401
13	1	1.466086	-0.016646	-1.491848
14	1	2.638180	-0.761429	-0.643185

2-mtea conformer 2

1	6	-1.801663	1.024035	-0.198651
2	16	-1.014812	-0.616599	-0.174869
3	1	-2.685463	0.938462	-0.826780
4	1	-1.143630	1.780205	-0.620920
5	1	-2.106876	1.317203	0.804769
6	6	0.366514	-0.301557	0.983182
7	6	1.476783	0.569984	0.415784
8	1	0.760159	-1.288642	1.222582
9	1	-0.042384	0.136407	1.893996
10	7	2.113211	-0.086819	-0.721917
11	1	2.228788	0.709407	1.196684
12	1	1.074188	1.565833	0.185560
13	1	2.828987	0.498757	-1.131244
14	1	1.422518	-0.279576	-1.438504

2-mtea conformer 3

1	6	-1.808235	1.173623	0.128820
2	16	-1.318913	-0.559810	-0.134088
3	1	-1.677508	1.453422	1.173213
4	1	-2.863710	1.242119	-0.124624
5	1	-1.250045	1.853123	-0.510905
6	6	0.401394	-0.514604	0.478495
7	6	1.383036	0.220796	-0.435553
8	1	0.693224	-1.561123	0.576790

9	1	0.404815	-0.078956	1.480124
10	7	2.765400	0.241729	0.037643
11	1	1.061009	1.254113	-0.568440
12	1	1.362317	-0.239649	-1.423763
13	1	3.130772	-0.696670	0.144917
14	1	2.840107	0.698467	0.938323

2-mtea conformer 4

1	6	1.618491	1.089064	0.410224
2	16	1.069550	-0.453718	-0.392592
3	1	1.943084	0.890536	1.429952
4	1	0.826551	1.832632	0.413383
5	1	2.464725	1.456466	-0.166404
6	6	-0.397341	-0.868997	0.629480
7	6	-1.719124	-0.428547	0.017588
8	1	-0.254399	-0.413510	1.608394
9	1	-0.389035	-1.951282	0.752574
10	7	-1.755628	1.019719	-0.185130
11	1	-2.520458	-0.694806	0.711525
12	1	-1.887620	-0.999274	-0.904888
13	1	-2.677382	1.316255	-0.478702
14	1	-1.113087	1.270661	-0.928037

2-mtea conformer 5

1	6	2.377001	-0.196903	0.466795
2	16	0.882629	0.456218	-0.335556
3	1	2.217627	-0.324518	1.536365
4	1	3.168833	0.532030	0.310257
5	1	2.674483	-1.144690	0.021266
6	6	-0.286548	-0.897711	0.046503
7	6	-1.713090	-0.498358	-0.338737
8	1	-0.231243	-1.112040	1.115787
9	1	0.016721	-1.791659	-0.501487

10	7	-2.312576	0.588198	0.427138
11	1	-2.351035	-1.378379	-0.234541
12	1	-1.736595	-0.223973	-1.395464
13	1	-1.740914	1.422373	0.372161
14	1	-2.379691	0.342498	1.407501

2-mtea conformer 6

1	6	2.334211	-0.143965	-0.540509
2	16	0.883855	0.407535	0.405482
3	1	2.651513	-1.135410	-0.221548
4	1	3.134722	0.564792	-0.341348
5	1	2.119010	-0.148641	-1.607650
6	6	-0.306989	-0.901310	-0.072947
7	6	-1.720864	-0.498127	0.315112
8	1	-0.026910	-1.830085	0.423500
9	1	-0.249785	-1.039778	-1.152516
10	7	-2.194188	0.602804	-0.523230
11	1	-1.748085	-0.280604	1.391711
12	1	-2.375244	-1.356319	0.148317
13	1	-1.581910	1.404632	-0.431358
14	1	-3.123542	0.894289	-0.250271

2-mtea conformer 7

1	6	-1.809441	1.166805	0.151940
2	16	-1.310621	-0.558054	-0.145567
3	1	-2.866178	1.233864	-0.096845
4	1	-1.257128	1.861416	-0.476866
5	1	-1.675231	1.427313	1.200647
6	6	0.406432	-0.514351	0.466251
7	6	1.374635	0.235512	-0.439892
8	1	0.701699	-1.561584	0.548245
9	1	0.423045	-0.090748	1.470311
10	7	2.716610	0.220307	0.148161
11	1	1.063750	1.277576	-0.521402

12	1	1.321189	-0.194657	-1.446740
13	1	3.345186	0.827532	-0.361587
14	1	3.113914	-0.710962	0.120599

2-mtea conformer 8

1	6	-1.824911	1.169012	0.114520
2	16	-1.307642	-0.559384	-0.128477
3	1	-1.717967	1.456073	1.159644
4	1	-2.876079	1.222862	-0.159912
5	1	-1.262018	1.851508	-0.518028
6	6	0.406767	-0.487379	0.488542
7	6	1.386322	0.182300	-0.466000
8	1	0.707311	-1.520145	0.657965
9	1	0.404115	0.014052	1.458764
10	7	2.731612	0.169841	0.115560
11	1	1.027138	1.188029	-0.715463
12	1	1.412437	-0.384648	-1.396485
13	1	2.791147	0.795951	0.909432
14	1	3.422236	0.475572	-0.557724

2-mtea conformer 9

1	6	1.650308	1.092250	0.390021
2	16	1.079699	-0.453574	-0.386908
3	1	0.915014	1.887531	0.294780
4	1	2.559249	1.385350	-0.131085
5	1	1.884080	0.927476	1.440329
6	6	-0.384695	-0.854724	0.640958
7	6	-1.718470	-0.431629	0.020455
8	1	-0.239582	-0.392059	1.618214
9	1	-0.370257	-1.935614	0.786365
10	7	-1.888973	0.986603	-0.265091
11	1	-2.522833	-0.745999	0.691446
12	1	-1.860721	-0.977177	-0.913748
13	1	-1.183447	1.296955	-0.922209

14	1	-1.795540	1.545583	0.574137
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2-mtea conformer 10

1	6	-2.402292	0.751446	0.000050
2	16	-1.152855	-0.569641	-0.000016
3	1	-2.312366	1.370791	0.891071
4	1	-3.377332	0.269525	0.000545
5	1	-2.313003	1.370230	-0.891424
6	6	0.361918	0.455243	-0.000094
7	6	1.606432	-0.432390	0.000065
8	1	0.355495	1.094452	0.884999
9	1	0.355540	1.094208	-0.885361
10	7	2.874531	0.291560	0.000027
11	1	1.587061	-1.084372	-0.874558
12	1	1.586993	-1.084165	0.874842
13	1	2.958779	0.885243	0.815874
14	1	2.958956	0.884824	-0.816105

2-mtea conformer 11

1	6	1.378731	1.298512	-0.223585
2	16	1.205157	-0.450485	0.253788
3	1	1.403254	1.394138	-1.308524
4	1	2.331928	1.634042	0.180225
5	1	0.566626	1.888459	0.187756
6	6	-0.358405	-0.913070	-0.568165
7	6	-1.638723	-0.517324	0.156073
8	1	-0.316318	-1.999134	-0.652255
9	1	-0.347618	-0.513201	-1.584816
10	7	-1.854364	0.930946	0.134628
11	1	-1.564568	-0.829617	1.197875
12	1	-2.467890	-1.083263	-0.294517
13	1	-2.635233	1.188142	0.724135
14	1	-2.074058	1.246951	-0.802693

2-mtea conformer 12

1	6	-2.390186	0.754410	0.026821
2	16	-1.148180	-0.572014	-0.024193
3	1	-2.299240	1.404736	-0.841799
4	1	-2.294130	1.340639	0.939232
5	1	-3.367739	0.277974	0.011922
6	6	0.365966	0.449322	0.008420
7	6	1.599326	-0.441757	0.030222
8	1	0.356048	1.087371	0.891346
9	1	0.377282	1.088109	-0.877224
10	7	2.806781	0.387994	0.028344
11	1	1.549365	-1.148992	-0.807078
12	1	1.597760	-1.031640	0.947466
13	1	2.934962	0.837510	-0.870117
14	1	3.631101	-0.172846	0.200456

2-mtea conformer 13

1	6	2.430828	-0.288193	-0.137178
2	16	0.839656	0.550440	0.138109
3	1	3.212375	0.450580	0.026473
4	1	2.507255	-0.658267	-1.158765
5	1	2.569034	-1.110921	0.563385
6	6	-0.271009	-0.865838	-0.195869
7	6	-1.671663	-0.612106	0.335958
8	1	0.145042	-1.749565	0.288488
9	1	-0.298153	-1.053344	-1.272019
10	7	-2.244807	0.601861	-0.239678
11	1	-1.622594	-0.476693	1.417423
12	1	-2.268295	-1.516384	0.147758
13	1	-3.158951	0.797389	0.145580
14	1	-2.345073	0.521764	-1.244166

2-mtea conformer 14

1	6	1.389525	1.185512	0.462721
2	16	1.132318	-0.392362	-0.399764
3	1	2.312990	1.605299	0.070239
4	1	1.500798	1.034226	1.535605
5	1	0.569112	1.868903	0.256097
6	6	-0.351013	-1.018565	0.465370
7	6	-1.518103	-0.047590	0.602023
8	1	-0.069326	-1.373825	1.457219
9	1	-0.649537	-1.890201	-0.119588
10	7	-1.845770	0.622486	-0.652513
11	1	-1.266931	0.718098	1.339331
12	1	-2.353837	-0.622382	1.025305
13	1	-1.854148	-0.026676	-1.428968
14	1	-2.754403	1.063574	-0.605765