

Supporting Information

Paper:

EPR spectrum of the Y@C₈₂ metallofullerene isolated in solid argon matrix: hyperfine structure from EPR spectroscopy and relativistic DFT calculations

Authors:

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Calculated structures and vibrational frequencies of endometallofullerenes Sc@C₈₂, Y@C₈₂, and La@C₈₂.

1.===== Sc@C₈₂ scalar relativistic PBE/L2//PBE/L2 =====

Atomic Coordinates:

21	0.07997313	2.30834246	-0.00799871
6	3.85104996	1.18380877	-1.21053456
6	3.70571567	1.90298833	0.00377382
6	2.81274859	3.02814281	-0.00156002
6	3.84379995	1.18958949	1.22233018
6	4.03791956	-0.22813592	1.22340909
6	4.05242657	-0.98086070	0.01165685
6	4.04515405	-0.23390044	-1.20372045
6	3.05231417	1.54825592	2.38467186
6	2.14738253	2.63238887	2.35234286
6	2.07290685	3.43311483	1.15264158
6	0.95220796	2.51325881	3.10522851
6	2.82251904	-1.99746449	2.41057412
6	3.38534738	-0.73724560	2.40516991
6	2.72128488	0.33729651	3.08968272
6	1.44384241	0.14602306	3.69357342
6	0.60226882	1.29439436	3.76197407
6	2.88764044	-2.82543851	-1.19309286
6	3.45671693	-2.32142516	0.01306764
6	2.88045109	-2.81970794	1.21819601
6	-0.26523053	3.15408523	2.64803223
6	-0.32911869	3.99030198	1.48619450
6	0.90581898	4.19288443	0.73199799
6	-1.54659506	3.89959964	0.71540202
6	-1.36641747	2.32697635	3.08701346
6	-3.28648637	1.03420298	2.36749441
6	-2.56716318	2.25112586	2.33109964
6	-2.63122282	3.04503003	1.13937080
6	1.57864376	-2.23707052	3.09541067
6	0.81833861	-1.17646749	3.66605198
6	-0.64405395	-1.29345558	3.66091254
6	-1.47498478	-0.08750802	3.68272756
6	-0.83050243	1.17966825	3.75152514
6	-2.76414540	-0.10446791	3.07165989
6	-1.54222533	3.89611698	-0.74863941
6	-0.32017294	3.98316170	-1.51257330
6	0.91024032	4.18934009	-0.75199396
6	-0.24937417	3.14144549	-2.67002960

6	-2.62431781	3.03952993	-1.17500777
6	-3.27227599	1.02287955	-2.39745523
6	-2.55316461	2.23997053	-2.36254841
6	-1.34793147	2.31224571	-3.11163728
6	-4.00585157	0.55544176	1.19984605
6	-3.98651551	1.28910488	-0.01770674
6	-3.30956981	2.55420228	-0.01869362
6	-3.99859879	0.54966601	-1.23185463
6	0.97076180	2.49847086	-3.11690925
6	2.16142307	2.62118815	-2.35747637
6	2.07979842	3.42760038	-1.16206157
6	3.06652197	1.53693243	-2.37926484
6	0.62472931	1.27649803	-3.76993682
6	1.46586552	0.12847737	-3.69106384
6	2.73968677	0.32263184	-3.08048358
6	2.83683525	-2.00887541	-2.38969324
6	3.39963914	-0.74863689	-2.38692211
6	-1.20153429	-2.47629917	-3.08796310
6	-0.62221024	-1.31086066	-3.66401958
6	0.84018983	-1.19387726	-3.66099012
6	1.59706201	-2.25174902	-3.08079348
6	-0.80807973	1.16180218	-3.76748690
6	-2.74576203	-0.11911694	-3.09307590
6	-1.45297978	-0.10504213	-3.69651721
6	-1.11137442	-3.88455617	-1.19934796
6	-0.40608822	-3.44776096	-2.38927771
6	0.96461438	-3.33855299	-2.38617193
6	-1.11854583	-3.87884748	1.20563246
6	-0.40409178	-4.14491374	0.00588580
6	-3.22684031	-1.28391676	-2.40233852
6	-2.40060625	-3.24551043	1.20288370
6	-3.04461868	-2.84588612	-0.00507280
6	-2.39341917	-3.25123189	-1.20725433
6	-2.46834884	-2.43607938	-2.40272850
6	-2.48266022	-2.42468348	2.39399937
6	-3.24111450	-1.27254377	2.38360816
6	-3.96326042	-0.87433666	1.19942674
6	-3.85042000	-1.62115602	-0.01038900
6	-3.95602971	-0.88009329	-1.22439058
6	0.95033305	-3.32716995	2.40220425
6	-0.42036457	-3.43638180	2.39765371
6	-1.21995136	-2.46162242	3.08695475
6	1.72445715	-3.65725704	-1.19196287
6	1.06153916	-4.02697794	0.00997744
6	1.71728081	-3.65154105	1.21408089

#

Vibrational frequencies

freq.	55.6	64.0	196.1	209.6	211.6	214.1
freq.	219.5	261.0	269.8	271.9	273.0	275.1
freq.	285.9	294.9	323.5	328.0	336.2	339.5
freq.	340.6	343.1	348.1	351.5	353.6	356.1
freq.	361.1	361.7	376.3	379.0	402.0	413.4
freq.	414.1	426.7	432.6	437.4	442.4	449.1

freq.	454.3	466.5	467.5	472.3	478.1	480.0
freq.	482.6	487.7	491.2	492.0	496.5	498.1
freq.	499.6	505.3	509.9	511.0	513.8	517.4
freq.	519.0	522.4	534.5	560.0	569.3	574.3
freq.	588.3	589.0	589.5	591.9	611.4	613.1
freq.	615.0	622.7	623.9	627.5	630.5	639.8
freq.	644.2	647.3	649.4	652.0	652.3	660.1
freq.	664.7	669.8	672.6	674.5	682.9	683.2
freq.	685.8	686.3	689.3	690.7	691.4	699.5
freq.	709.3	711.5	714.1	716.9	718.2	724.1
freq.	724.8	728.5	729.5	735.4	738.4	742.6
freq.	744.7	751.3	754.3	755.6	760.7	765.4
freq.	766.3	767.8	772.2	772.5	775.9	777.1
freq.	789.0	790.2	790.3	791.8	792.7	793.3
freq.	797.1	797.9	801.7	824.2	829.0	836.9
freq.	847.9	859.1	861.6	867.5	868.7	874.2
freq.	875.0	879.4	887.6	920.6	1003.4	1005.6
freq.	1007.6	1014.8	1015.4	1021.5	1025.2	1032.4
freq.	1036.4	1107.9	1114.7	1117.5	1120.5	1124.7
freq.	1133.9	1136.6	1140.3	1156.8	1158.9	1160.9
freq.	1174.7	1178.1	1186.9	1190.7	1199.7	1201.8
freq.	1206.0	1213.4	1213.6	1224.8	1228.2	1230.4
freq.	1239.8	1245.0	1254.2	1256.5	1260.4	1264.2
freq.	1265.0	1269.9	1271.1	1273.6	1280.7	1294.0
freq.	1306.6	1308.1	1308.7	1315.1	1315.4	1318.5
freq.	1320.8	1324.8	1328.6	1332.1	1332.7	1334.0
freq.	1338.0	1340.4	1349.8	1351.2	1353.8	1364.0
freq.	1364.0	1368.4	1370.6	1372.9	1375.5	1379.0
freq.	1379.7	1381.7	1395.2	1401.5	1407.2	1412.7
freq.	1412.9	1416.0	1422.8	1423.4	1426.8	1432.7
freq.	1433.9	1436.0	1441.8	1443.4	1451.9	1456.8
freq.	1462.9	1469.5	1476.1	1476.5	1482.4	1490.0
freq.	1491.9	1492.5	1508.1	1509.7	1511.6	1514.9
freq.	1516.4	1516.6	1517.8	1562.6	1573.0	1579.6
freq.	1580.3	1603.8	1610.9			

2. ===== Y@C₈₂ scalar relativistic PBE/L2//PBE/L2 =====

Atomic Coordinates:

39	0.03106681	2.14675248	-0.00771740
6	3.85322368	1.18547532	-1.21031498
6	3.70833145	1.90559244	0.00377637
6	2.82028283	3.03711848	-0.00156045
6	3.84597128	1.19125250	1.22211743
6	4.03869107	-0.22752593	1.22315332
6	4.05341602	-0.98063572	0.01166302
6	4.04592711	-0.23328987	-1.20345780
6	3.05380546	1.54988103	2.38415058
6	2.14987249	2.63622714	2.35107597
6	2.08083010	3.44164223	1.15399766
6	0.95168815	2.51653733	3.10106563
6	2.82246588	-1.99711716	2.41048751
6	3.38530566	-0.73623920	2.40408979
6	2.72124041	0.33864791	3.08821364
6	1.44348538	0.14731635	3.69164827
6	0.60149815	1.29554473	3.75874206
6	2.88753324	-2.82520239	-1.19308853
6	3.45694670	-2.32110635	0.01306908
6	2.88034263	-2.81947358	1.21819065
6	-0.26589234	3.16192298	2.65046365
6	-0.33016185	4.00209275	1.48911999
6	0.90547185	4.18556640	0.73141284
6	-1.55170270	3.91794768	0.71769665
6	-1.36667354	2.33035412	3.08889311
6	-3.28578612	1.03606976	2.36744077
6	-2.56699362	2.25366420	2.33286964
6	-2.62855762	3.05019628	1.13975880
6	1.57904938	-2.23656432	3.09504989
6	0.81813251	-1.17543131	3.66525332
6	-0.64402355	-1.29264244	3.66052571
6	-1.47473513	-0.08698231	3.68222359
6	-0.82960953	1.18129012	3.75140258
6	-2.76366956	-0.10383675	3.07185985
6	-1.54732068	3.91445143	-0.75105745
6	-0.32119792	3.99493286	-1.51556704
6	0.90989215	4.18203411	-0.75138677
6	-0.25001677	3.14925823	-2.67249720
6	-2.62165177	3.04469462	-1.17541015
6	-3.27157722	1.02474941	-2.39740817
6	-2.55298715	2.24250626	-2.36433690
6	-1.34818442	2.31562923	-3.11355582
6	-4.00439507	0.55681017	1.20007305
6	-3.98225299	1.28900843	-0.01769550
6	-3.30263237	2.55382362	-0.01867320
6	-3.99714224	0.55103240	-1.23208193
6	0.97021923	2.50177843	-3.11278401
6	2.16390708	2.62504193	-2.35622523
6	2.08773632	3.43612954	-1.16341713
6	3.06800731	1.53856467	-2.37874469
6	0.62393676	1.27766451	-3.76671648

6	1.46549329	0.12977970	-3.68914483
6	2.73963129	0.32399463	-3.07901587
6	2.83677968	-2.00852117	-2.38960347
6	3.39958991	-0.74761911	-2.38584067
6	-1.20212610	-2.47651257	-3.08798067
6	-0.62218342	-1.31004424	-3.66363245
6	0.83997619	-1.19283637	-3.66019457
6	1.59746452	-2.25123620	-3.08042547
6	-0.80719050	1.16342788	-3.76736847
6	-2.74528678	-0.11848520	-3.09327643
6	-1.45273407	-0.10451148	-3.69601351
6	-1.11153954	-3.88534274	-1.19945185
6	-0.40619151	-3.44776506	-2.38929804
6	0.96450378	-3.33825225	-2.38597014
6	-1.11871120	-3.87962850	1.20573692
6	-0.40430056	-4.14548657	0.00588743
6	-3.22652387	-1.28325958	-2.40253246
6	-2.40055805	-3.24569569	1.20300216
6	-3.04415205	-2.84584795	-0.00507300
6	-2.39337069	-3.25142302	-1.20737486
6	-2.46830891	-2.43636581	-2.40339202
6	-2.48261643	-2.42496566	2.39466433
6	-3.24079588	-1.27188693	2.38380272
6	-3.96243666	-0.87371838	1.19973363
6	-3.84946337	-1.62016939	-0.01038712
6	-3.95520747	-0.87947815	-1.22469343
6	0.95022660	-3.32687686	2.40200462
6	-0.42046590	-3.43639196	2.39767657
6	-1.22053891	-2.46184125	3.08697545
6	1.72439382	-3.65748161	-1.19194406
6	1.06154105	-4.02738790	0.00997881
6	1.71721898	-3.65176536	1.21406310

#

Vibrational frequencies

freq.	35.8	37.1	176.5	208.3	211.9	214.4
freq.	220.0	249.0	270.4	271.9	273.4	275.1
freq.	286.3	295.1	323.6	323.8	328.2	339.8
freq.	340.3	344.6	348.6	352.1	353.1	356.6
freq.	361.1	362.1	375.0	378.8	395.7	412.3
freq.	418.0	422.8	431.1	437.4	442.9	448.0
freq.	455.0	464.9	465.0	472.4	477.6	479.7
freq.	482.6	487.9	491.0	492.1	495.7	497.9
freq.	499.1	505.0	510.4	511.0	513.4	517.4
freq.	519.2	522.8	532.8	553.8	567.5	569.8
freq.	583.8	588.5	588.8	591.7	611.4	613.3
freq.	615.4	622.9	624.8	626.3	631.1	639.4
freq.	644.3	646.9	649.6	652.1	652.6	659.8
freq.	664.6	670.1	671.1	673.0	681.5	683.3
freq.	686.0	687.1	688.2	690.2	691.9	699.8
freq.	711.8	712.5	714.7	717.0	718.1	724.9
freq.	725.3	728.4	729.1	733.5	738.3	742.3
freq.	745.4	751.0	754.6	755.6	760.6	765.8
freq.	766.8	768.1	772.0	772.6	776.7	777.3

freq.	790.0	790.7	792.0	792.8	793.0	793.4
freq.	796.9	798.4	802.1	824.0	827.3	836.8
freq.	847.7	858.7	861.8	867.3	868.6	874.6
freq.	875.1	877.7	886.7	920.5	1002.4	1005.6
freq.	1006.9	1014.5	1015.7	1020.7	1025.0	1031.9
freq.	1036.0	1108.1	1115.0	1115.3	1120.5	1124.7
freq.	1133.7	1136.0	1139.3	1156.9	1158.7	1160.0
freq.	1175.5	1177.2	1186.1	1190.3	1198.5	1201.8
freq.	1206.3	1211.4	1213.0	1224.0	1228.0	1229.5
freq.	1239.7	1245.1	1254.7	1256.6	1261.0	1264.5
freq.	1265.4	1269.4	1270.6	1273.7	1279.0	1293.3
freq.	1305.9	1306.0	1308.2	1315.3	1315.3	1317.9
freq.	1319.1	1325.5	1328.3	1330.6	1332.9	1333.0
freq.	1337.6	1340.0	1350.0	1350.7	1353.2	1359.0
freq.	1363.4	1365.7	1367.4	1369.0	1375.4	1378.0
freq.	1378.8	1379.5	1394.8	1399.5	1405.2	1409.9
freq.	1412.7	1416.5	1421.2	1422.7	1427.1	1430.9
freq.	1432.6	1433.3	1440.4	1443.4	1450.6	1454.9
freq.	1461.7	1469.0	1475.2	1475.9	1482.2	1489.2
freq.	1490.4	1491.8	1507.6	1509.7	1510.7	1514.4
freq.	1515.8	1516.0	1517.2	1561.5	1572.3	1577.4
freq.	1578.9	1603.3	1610.5			

3. ===== La@C₈₂ scalar relativistic PBE/L2//PBE/L2 =====
Atomic Coordinates:

57	-0.03238721	1.95095813	-0.00743242
6	3.85599945	1.18841624	-1.21016969
6	3.71444118	1.91124559	0.00378899
6	2.83541809	3.05085587	-0.00155714
6	3.84882112	1.19427170	1.22203760
6	4.03914847	-0.22522730	1.22261078
6	4.05409679	-0.97899467	0.01167658
6	4.04638448	-0.23103904	-1.20290554
6	3.05610480	1.55272743	2.38446133
6	2.15380408	2.64172893	2.35087996
6	2.09185538	3.44773961	1.15510623
6	0.95266117	2.52269597	3.09985718
6	2.82250651	-1.99529871	2.41007353
6	3.38546681	-0.73410852	2.40310316
6	2.72197414	0.34126704	3.08719494
6	1.44355187	0.14992132	3.68912381
6	0.60170514	1.29825483	3.75453829
6	2.88762049	-2.82383786	-1.19297492
6	3.45725659	-2.31943955	0.01306221
6	2.88041877	-2.81806749	1.21805239
6	-0.26645834	3.17261260	2.65911325
6	-0.33017270	4.00209784	1.48988768
6	0.90247885	4.16174470	0.72888627
6	-1.55458092	3.92639123	0.71874042
6	-1.36747860	2.33612321	3.09211256
6	-3.28522130	1.03927638	2.36743716
6	-2.56804910	2.25838953	2.33495625
6	-2.63112597	3.05728760	1.14076371
6	1.57948466	-2.23481524	3.09449808
6	0.81827608	-1.17307018	3.66384982
6	-0.64359770	-1.29065453	3.65943744
6	-1.47390800	-0.08503958	3.68065366
6	-0.82851523	1.18382884	3.74976111
6	-2.76316533	-0.10177981	3.07165024
6	-1.55015204	3.92286565	-0.75208608
6	-0.32120489	3.99499743	-1.51632145
6	0.90689989	4.15822741	-0.74879048
6	-0.25057119	3.15982942	-2.68107907
6	-2.62413372	3.05171006	-1.17642852
6	-3.27104532	1.02795346	-2.39742176
6	-2.55407085	2.24722474	-2.36648135
6	-1.34899108	2.32134816	-3.11678300
6	-4.00346437	0.55950265	1.20016756
6	-3.98125056	1.29123922	-0.01770397
6	-3.30331349	2.55825052	-0.01868778
6	-3.99621421	0.55370329	-1.23219155
6	0.97113858	2.50788469	-3.11147124
6	2.16778925	2.63043768	-2.35595786
6	2.09875238	3.44217773	-1.16449359
6	3.07017940	1.54122310	-2.37893547

6	0.62410928	1.28039153	-3.76250417
6	1.46551682	0.13237752	-3.68665422
6	2.74031916	0.32651618	-3.07798746
6	2.83685385	-2.00677682	-2.38924328
6	3.39976490	-0.74557089	-2.38486268
6	-1.20221502	-2.47540273	-3.08770534
6	-0.62177241	-1.30806346	-3.66256151
6	0.84010271	-1.19049010	-3.65884192
6	1.59791276	-2.24952622	-3.07993859
6	-0.80612110	1.16596465	-3.76574290
6	-2.74481027	-0.11642136	-3.09311320
6	-1.45192821	-0.10256846	-3.69447336
6	-1.11159283	-3.88511406	-1.19963067
6	-0.40612966	-3.44692695	-2.38938301
6	0.96473073	-3.33686178	-2.38584236
6	-1.11875396	-3.87938143	1.20587875
6	-0.40430795	-4.14525548	0.00587072
6	-3.22598676	-1.28121537	-2.40250134
6	-2.40027054	-3.24467886	1.20306199
6	-3.04349784	-2.84450891	-0.00508630
6	-2.39309422	-3.25040742	-1.20747547
6	-2.46790882	-2.43509283	-2.40359964
6	-2.48221106	-2.42368627	2.39482820
6	-3.24025213	-1.26984162	2.38371999
6	-3.96141472	-0.87156914	1.19974007
6	-3.84840066	-1.61797950	-0.01039596
6	-3.95418989	-0.87735542	-1.22473505
6	0.95045059	-3.32546193	2.40183358
6	-0.42040301	-3.43552681	2.39772423
6	-1.22061623	-2.46071010	3.08665706
6	1.72476102	-3.65657598	-1.19193408
6	1.06184049	-4.02692823	0.00996657
6	1.71758284	-3.65082907	1.21402203

#

Vibrational frequencies

freq.	23.6	24.0	157.1	208.3	212.3	214.4
freq.	220.2	243.1	271.0	273.8	274.5	276.3
freq.	286.0	294.3	316.5	323.9	328.2	339.9
freq.	341.7	346.4	348.5	354.2	355.8	357.4
freq.	362.6	364.6	374.3	377.3	394.1	414.3
freq.	422.0	425.7	432.9	439.7	444.6	452.7
freq.	457.2	463.5	464.7	473.3	478.2	480.5
freq.	483.6	488.2	491.0	493.9	495.5	498.8
freq.	499.3	504.8	510.8	512.6	513.4	517.1
freq.	519.9	522.4	529.5	545.9	565.8	568.1
freq.	583.0	588.4	588.5	591.4	611.4	613.4
freq.	615.2	623.0	625.6	626.5	631.9	639.6
freq.	644.5	646.6	650.1	652.1	653.0	659.3
freq.	663.7	668.1	669.8	673.2	681.2	683.2
freq.	685.5	686.1	687.6	689.9	691.7	700.1
freq.	712.1	714.7	715.2	717.2	717.6	725.2
freq.	726.2	726.8	727.9	732.2	737.8	742.2
freq.	742.4	750.6	753.1	755.4	760.8	764.9

freq.	766.5	768.4	770.8	772.4	776.7	777.4
freq.	790.1	790.9	792.1	792.3	793.1	793.2
freq.	796.7	798.9	802.5	824.2	826.2	836.6
freq.	847.8	858.1	861.7	866.8	868.9	874.6
freq.	875.1	876.9	886.3	920.4	1002.8	1005.4
freq.	1006.3	1014.9	1015.9	1019.9	1025.1	1031.1
freq.	1035.6	1110.1	1113.8	1115.4	1120.6	1124.9
freq.	1133.8	1135.3	1138.9	1157.2	1159.5	1160.9
freq.	1175.3	1176.5	1185.3	1189.2	1197.9	1201.7
freq.	1206.1	1210.6	1213.1	1222.9	1227.3	1229.5
freq.	1240.8	1244.4	1254.3	1256.8	1261.3	1263.6
freq.	1266.5	1269.2	1269.5	1273.2	1278.4	1293.2
freq.	1305.6	1306.5	1307.2	1315.2	1316.4	1317.6
freq.	1320.9	1326.5	1328.0	1329.4	1333.6	1334.8
freq.	1337.2	1339.7	1350.0	1350.4	1352.9	1356.0
freq.	1362.3	1362.5	1364.1	1366.4	1374.7	1376.9
freq.	1378.1	1378.7	1393.6	1397.1	1404.8	1408.2
freq.	1412.6	1416.3	1419.9	1421.3	1427.1	1428.3
freq.	1430.4	1431.7	1438.9	1442.7	1449.4	1453.6
freq.	1460.1	1467.9	1474.4	1475.1	1481.3	1487.5
freq.	1489.0	1490.9	1506.7	1507.9	1508.5	1513.2
freq.	1514.5	1515.1	1516.3	1560.3	1571.5	1575.8
freq.	1577.7	1602.4	1609.8			

4. ===== Sc@C₈₂ scalar relativistic PBE/r3zv//PBE/r3zv

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Atomic Coordinates:

21	0.08132870	2.32260335	-0.00803229
6	3.84527178	1.18189954	-1.20885284
6	3.69905132	1.90024167	0.00375744
6	2.80339092	3.02083697	-0.00157359
6	3.83801794	1.18766617	1.22061528
6	4.03600767	-0.22879275	1.22289137
6	4.04544875	-0.97989347	0.01163222
6	4.04324728	-0.23455121	-1.20322088
6	3.04878367	1.54652646	2.38192218
6	2.14365261	2.62894854	2.34853372
6	2.06733460	3.42920684	1.15095339
6	0.95091928	2.50933745	3.10056200
6	2.82101992	-1.99672178	2.40916367
6	3.38392262	-0.73714464	2.40410069
6	2.71894154	0.33630352	3.08715151
6	1.44138351	0.14486084	3.68723629
6	0.60187524	1.29248158	3.75986737
6	2.88538845	-2.82300796	-1.19233534
6	3.45306781	-2.31914460	0.01305234
6	2.87819738	-2.81730618	1.21741184
6	-0.26437037	3.14803998	2.64055794
6	-0.32901805	3.99308127	1.48592751
6	0.90607290	4.19976066	0.73285941
6	-1.54561926	3.90275208	0.71518241
6	-1.36425498	2.32331709	3.08197482
6	-3.28336156	1.03300100	2.36504573
6	-2.56222622	2.24739953	2.32638872
6	-2.62529885	3.04135806	1.13758598
6	1.57787361	-2.23626051	3.09361206
6	0.81717417	-1.17534081	3.66066874
6	-0.64307178	-1.29202078	3.65511863
6	-1.47257168	-0.08818458	3.67687212
6	-0.82960238	1.17771727	3.74872277
6	-2.76189287	-0.10508549	3.06915139
6	-1.54125323	3.89927497	-0.74843737
6	-0.32007519	3.98595833	-1.51233229
6	0.91050459	4.19623158	-0.75290156
6	-0.24855368	3.13544327	-2.66252976
6	-2.61840711	3.03586889	-1.17317465
6	-3.26916474	1.02169405	-2.39498102
6	-2.54825613	2.23627281	-2.35779420
6	-1.34579827	2.30861738	-3.10657403
6	-4.00113274	0.55445455	1.19843735
6	-3.98070549	1.28728260	-0.01768636
6	-3.30197869	2.54939171	-0.01866074
6	-3.99388818	0.54868499	-1.23041436
6	0.96944831	2.49458152	-3.11223827
6	2.15767793	2.61778273	-2.35368751
6	2.07422779	3.42371796	-1.16039725
6	3.06297854	1.53522878	-2.37653487

6	0.62432441	1.27460248	-3.76782522
6	1.46336458	0.12735103	-3.68473185
6	2.73732409	0.32166610	-3.07795980
6	2.83532316	-2.00810974	-2.38828934
6	3.39818691	-0.74851266	-2.38585037
6	-1.20097271	-2.47537153	-3.08623720
6	-0.62126128	-1.30939381	-3.65822270
6	0.83899202	-1.19271950	-3.65561394
6	1.59627867	-2.25091761	-3.07898519
6	-0.80719487	1.15987143	-3.76467097
6	-2.74352186	-0.11971703	-3.09054872
6	-1.45059883	-0.10568466	-3.69064200
6	-1.11026592	-3.88199671	-1.19876001
6	-0.40599223	-3.44560584	-2.38755908
6	0.96426104	-3.33664366	-2.38461030
6	-1.11743644	-3.87629043	1.20504465
6	-0.40329369	-4.13897652	0.00588005
6	-3.22542562	-1.28350757	-2.40110386
6	-2.39878724	-3.24269774	1.20209584
6	-3.04128908	-2.84275566	-0.00507058
6	-2.39160516	-3.24841792	-1.20646905
6	-2.46686080	-2.43495806	-2.40114282
6	-2.48115905	-2.42357261	2.39241960
6	-3.23969216	-1.27214431	2.38238148
6	-3.96160832	-0.87474187	1.19899898
6	-3.84435097	-1.61921849	-0.01037397
6	-3.95438099	-0.88049814	-1.22394930
6	0.94998979	-3.32528060	2.40065141
6	-0.42025795	-3.43424049	2.39593344
6	-1.21937989	-2.46071003	3.08523528
6	1.72306977	-3.65507086	-1.19141052
6	1.05986036	-4.02120258	0.00996726
6	1.71588314	-3.64934559	1.21352125

#

Vibrational frequencies

freq.	59.4	65.3	197.1	209.6	211.4	214.6
freq.	219.9	262.5	269.6	270.4	272.7	274.3
freq.	285.8	295.2	322.7	327.5	336.4	338.8
freq.	338.9	341.2	347.6	348.8	350.4	353.7
freq.	358.1	359.3	374.3	377.7	402.8	404.3
freq.	407.7	422.2	424.4	430.3	436.7	442.5
freq.	446.6	458.2	461.1	465.7	469.1	474.7
freq.	475.7	483.9	485.2	486.5	490.1	493.2
freq.	496.6	499.7	501.0	505.3	506.8	511.4
freq.	517.8	521.3	531.1	547.8	556.9	558.5
freq.	584.1	588.9	590.0	592.2	595.9	604.6
freq.	606.9	612.0	612.6	616.6	623.1	624.3
freq.	625.8	627.4	630.5	630.7	637.5	641.4
freq.	643.3	645.9	648.2	653.5	656.1	657.3
freq.	657.9	660.5	664.9	665.7	667.1	669.0
freq.	671.9	672.7	674.2	675.7	676.0	676.3
freq.	678.3	680.4	680.9	681.0	684.7	686.8
freq.	687.7	688.2	690.3	692.8	693.8	694.2

freq.	698.2	700.3	710.6	713.3	715.6	725.9
freq.	736.3	738.2	744.2	748.8	757.2	773.8
freq.	774.8	789.6	790.0	824.7	829.4	835.4
freq.	849.6	860.1	863.1	867.5	869.6	872.6
freq.	876.3	880.2	889.0	913.2	1005.0	1007.7
freq.	1010.5	1017.7	1018.1	1024.5	1026.7	1035.7
freq.	1038.5	1110.4	1117.3	1120.9	1123.9	1130.0
freq.	1140.0	1140.3	1146.1	1160.9	1163.7	1165.7
freq.	1181.3	1184.7	1191.8	1195.9	1204.8	1206.3
freq.	1214.9	1218.4	1221.9	1233.7	1235.0	1237.6
freq.	1246.0	1253.7	1260.1	1261.4	1267.1	1272.4
freq.	1272.8	1276.0	1277.3	1281.8	1287.3	1298.8
freq.	1315.0	1316.3	1318.2	1323.1	1323.8	1325.6
freq.	1327.8	1332.4	1338.5	1339.7	1340.9	1345.0
freq.	1351.8	1355.0	1363.9	1365.8	1368.2	1374.7
freq.	1378.3	1380.7	1382.5	1385.7	1390.2	1391.6
freq.	1391.6	1395.2	1412.0	1415.4	1419.6	1422.9
freq.	1424.5	1429.9	1432.9	1437.4	1437.5	1443.6
freq.	1447.8	1449.3	1454.8	1457.4	1466.2	1469.8
freq.	1475.1	1483.2	1486.5	1487.9	1496.4	1503.2
freq.	1503.3	1508.6	1521.3	1524.0	1525.8	1527.9
freq.	1529.1	1530.3	1532.3	1578.5	1588.6	1595.0
freq.	1595.8	1620.2	1626.6			

5. ===== Y@C₈₂ scalar relativistic PBE/r3zv//PBE/r3zv

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Atomic Coordinates:

39	0.03828010	2.16482095	-0.00774515
6	3.84619897	1.18339131	-1.20833715
6	3.70048271	1.90285538	0.00375838
6	2.81011600	3.03017102	-0.00157595
6	3.83895437	1.18916149	1.22010613
6	4.03605318	-0.22842383	1.22241207
6	4.04498610	-0.97990182	0.01163461
6	4.04328700	-0.23418585	-1.20273084
6	3.04947086	1.54824461	2.38090946
6	2.14602529	2.63339885	2.34735432
6	2.07510912	3.43917092	1.15254371
6	0.95048615	2.51326162	3.09648761
6	2.82091802	-1.99696497	2.40887129
6	3.38328453	-0.73641827	2.40254971
6	2.71826051	0.33747303	3.08488137
6	1.44038633	0.14603019	3.68362954
6	0.60099485	1.29388155	3.75573978
6	2.88533457	-2.82368466	-1.19235749
6	3.45294436	-2.31954899	0.01305116
6	2.87814736	-2.81796168	1.21743519
6	-0.26499018	3.15659097	2.64280947
6	-0.33034344	4.00750277	1.48977777
6	0.90584116	4.19623133	0.73268422
6	-1.55127576	3.92316303	0.71797515
6	-1.36444193	2.32708540	3.08348601
6	-3.28211060	1.03477764	2.36450589
6	-2.56238368	2.25067574	2.32834585
6	-2.62166951	3.04616957	1.13768245
6	1.57832598	-2.23659290	3.09305884
6	0.81665756	-1.17455747	3.65760738
6	-0.64289987	-1.29147630	3.65261195
6	-1.47168311	-0.08769854	3.67420588
6	-0.82866736	1.17960974	3.74778068
6	-2.76100055	-0.10468009	3.06854237
6	-1.54689213	3.91966481	-0.75137585
6	-0.32137365	4.00034251	-1.51626312
6	0.91026918	4.19269065	-0.75271133
6	-0.24915626	3.14397345	-2.66483360
6	-2.61479504	3.04069271	-1.17328492
6	-3.26791355	1.02348141	-2.39443399
6	-2.54840476	2.23954394	-2.35975600
6	-1.34597193	2.31236745	-3.10810230
6	-3.99891315	0.55555788	1.19845358
6	-3.97547158	1.28696737	-0.01766866
6	-3.29441659	2.54909373	-0.01863513
6	-3.99166888	0.54979303	-1.23041416
6	0.96899216	2.49851335	-3.10818477
6	2.16004111	2.62223278	-2.35251545
6	2.08200898	3.43366726	-1.16198815
6	3.06365520	1.53694417	-2.37552193

6	0.62342129	1.27601256	-3.76369956
6	1.46234841	0.12852618	-3.68112665
6	2.73662957	0.32283865	-3.07569296
6	2.83522649	-2.00835885	-2.38800068
6	3.39756095	-0.74778756	-2.38431292
6	-1.20167363	-2.47648589	-3.08611394
6	-0.62110280	-1.30884023	-3.65572641
6	0.83845945	-1.19192956	-3.65257329
6	1.59673835	-2.25125327	-3.07844368
6	-0.80626388	1.16176544	-3.76372302
6	-2.74263244	-0.11930562	-3.08993480
6	-1.44972529	-0.10518521	-3.68797555
6	-1.11052501	-3.88412357	-1.19897707
6	-0.40609354	-3.44679137	-2.38768056
6	0.96421140	-3.33757121	-2.38452231
6	-1.11769686	-3.87841267	1.20526180
6	-0.40351361	-4.14058904	0.00587748
6	-3.22491927	-1.28332297	-2.40094419
6	-2.39885831	-3.24385980	1.20224260
6	-3.04073022	-2.84353166	-0.00506350
6	-2.39167268	-3.24958455	-1.20661137
6	-2.46705241	-2.43606895	-2.40172524
6	-2.48134989	-2.42467668	2.39300591
6	-3.23918182	-1.27196016	2.38222867
6	-3.96047154	-0.87451671	1.19914683
6	-3.84237680	-1.61851423	-0.01036356
6	-3.95324753	-0.88027187	-1.22408132
6	0.94993731	-3.32620411	2.40054775
6	-0.42036330	-3.43542866	2.39605159
6	-1.22007795	-2.46182200	3.08510913
6	1.72320242	-3.65668843	-1.19154780
6	1.05992742	-4.02261975	0.00996179
6	1.71602771	-3.65097648	1.21365085

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Vibrational frequencies

freq.	34.0	39.4	178.5	207.9	211.6	214.9
freq.	220.5	250.1	269.7	269.7	272.9	274.3
freq.	286.1	295.3	322.8	324.6	327.6	337.8
freq.	339.0	342.2	347.7	348.5	349.3	353.2
freq.	358.2	358.5	372.4	376.8	395.6	402.0
freq.	409.6	419.1	421.1	428.2	435.9	440.4
freq.	446.1	454.4	458.5	464.1	465.4	474.1
freq.	474.2	482.5	482.8	484.4	489.2	492.7
freq.	496.8	497.3	499.0	504.9	505.9	511.3
freq.	517.4	521.8	530.3	542.7	553.0	557.3
freq.	571.0	588.4	589.5	591.2	596.0	601.5
freq.	603.7	611.4	612.2	617.3	620.5	621.6
freq.	624.4	624.5	625.9	627.8	628.8	638.6
freq.	643.2	644.4	646.7	648.0	653.7	654.5
freq.	654.7	658.1	663.6	666.1	666.3	667.0
freq.	667.7	669.2	671.1	672.4	673.3	674.3
freq.	675.0	677.9	679.2	679.9	681.3	682.4
freq.	682.6	686.4	687.1	688.1	690.9	691.7

freq.	692.6	697.1	711.9	717.1	718.2	729.6
freq.	736.2	739.7	745.0	752.1	768.2	773.5
freq.	775.1	789.5	789.8	824.5	827.5	834.8
freq.	849.1	859.4	863.3	867.8	868.8	873.2
freq.	876.8	878.0	887.4	913.1	1002.8	1007.1
freq.	1008.9	1016.9	1017.9	1023.3	1026.7	1034.8
freq.	1037.7	1109.7	1116.8	1117.9	1123.6	1129.2
freq.	1138.9	1139.0	1144.3	1160.7	1162.8	1163.8
freq.	1181.6	1183.2	1190.6	1195.0	1203.1	1205.2
freq.	1214.2	1215.2	1220.8	1232.0	1233.1	1237.0
freq.	1245.4	1252.8	1259.7	1260.9	1267.1	1271.5
freq.	1272.9	1275.8	1276.5	1281.1	1285.3	1297.7
freq.	1311.3	1315.1	1317.4	1322.4	1322.8	1323.8
freq.	1325.5	1331.8	1337.2	1338.3	1338.9	1344.0
freq.	1350.8	1354.6	1361.5	1365.3	1367.2	1367.3
freq.	1373.6	1376.4	1378.5	1383.2	1388.6	1390.0
freq.	1391.1	1393.5	1410.8	1413.0	1417.2	1420.8
freq.	1422.9	1429.1	1430.7	1436.4	1437.1	1440.5
freq.	1445.0	1446.9	1452.4	1457.0	1464.2	1467.1
freq.	1473.6	1482.1	1485.2	1486.3	1496.0	1501.5
freq.	1501.7	1506.7	1520.6	1524.1	1524.7	1526.7
freq.	1527.9	1529.5	1530.8	1576.4	1587.1	1591.8
freq.	1593.3	1618.6	1625.1			

6. ===== Sc@C₈₂ non-relativistic PBE/n3zv//PBE/n3zv

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Atomic Coordinates:

21	0.07874566	2.32051158	-0.00803640
6	3.84618551	1.18223806	-1.20913883
6	3.70020917	1.90083352	0.00376252
6	2.80464502	3.02173589	-0.00157069
6	3.83893742	1.18801146	1.22091393
6	4.03676500	-0.22872295	1.22313391
6	4.04621774	-0.97998657	0.01163940
6	4.04400250	-0.23448808	-1.20344587
6	3.04958821	1.54691619	2.38255936
6	2.14419524	2.62949738	2.34906266
6	2.06805873	3.42952381	1.15118904
6	0.95113315	2.50995789	3.10124997
6	2.82154167	-1.99699127	2.40958020
6	3.38456424	-0.73718774	2.40455765
6	2.71955654	0.33647005	3.08781531
6	1.44169019	0.14499172	3.68794315
6	0.60204171	1.29282844	3.76059777
6	2.88599877	-2.82350345	-1.19257642
6	3.45371471	-2.31946276	0.01305354
6	2.87880980	-2.81777372	1.21765770
6	-0.26451115	3.14893512	2.64163259
6	-0.32909797	3.99310722	1.48623864
6	0.90590997	4.19862441	0.73280843
6	-1.54579770	3.90292001	0.71529810
6	-1.36465556	2.32406737	3.08306377
6	-3.28401386	1.03334830	2.36560110
6	-2.56268011	2.24793868	2.32695878
6	-2.62607744	3.04216318	1.13796071
6	1.57816811	-2.23656880	3.09417338
6	0.81733935	-1.17544166	3.66133911
6	-0.64314515	-1.29211919	3.65576361
6	-1.47282468	-0.08808249	3.67764782
6	-0.82978378	1.17806018	3.74955636
6	-2.76238735	-0.10497958	3.06974372
6	-1.54143160	3.89944120	-0.74855363
6	-0.32015448	3.98598289	-1.51264404
6	0.91034088	4.19509500	-0.75284645
6	-0.24868993	3.13633077	-2.66360762
6	-2.61918238	3.03666925	-1.17355698
6	-3.26981535	1.02203606	-2.39553984
6	-2.54870756	2.23680653	-2.35836938
6	-1.34619406	2.30936033	-3.10766978
6	-4.00182362	0.55468812	1.19869541
6	-3.98155173	1.28764488	-0.01768800
6	-3.30271230	2.54997395	-0.01866350
6	-3.99457947	0.54891656	-1.23067444
6	0.96966489	2.49519272	-3.11292348
6	2.15822172	2.61832287	-2.35421126
6	2.07495368	3.42403152	-1.16062817
6	3.06378405	1.53560829	-2.37716382

6	0.62449464	1.27493984	-3.76855138
6	1.46367949	0.12747369	-3.68543771
6	2.73794667	0.32181961	-3.07861514
6	2.83585416	-2.00839228	-2.38870441
6	3.39885298	-0.74857015	-2.38630943
6	-1.20116812	-2.47570560	-3.08681007
6	-0.62133011	-1.30949626	-3.65886554
6	0.83916434	-1.19282714	-3.65628386
6	1.59658468	-2.25123751	-3.07955727
6	-0.80737326	1.16020634	-3.76550737
6	-2.74401510	-0.11961707	-3.09114237
6	-1.45084862	-0.10558950	-3.69141718
6	-1.11045705	-3.88265005	-1.19900630
6	-0.40606901	-3.44616849	-2.38801569
6	0.96447994	-3.33720450	-2.38508301
6	-1.11762670	-3.87694231	1.20528677
6	-0.40333224	-4.13965508	0.00587632
6	-3.22602584	-1.28361171	-2.40157288
6	-2.39924432	-3.24321287	1.20233145
6	-3.04182869	-2.84315145	-0.00507091
6	-2.39206120	-3.24893444	-1.20670561
6	-2.46730213	-2.43529711	-2.40158002
6	-2.48159837	-2.42390737	2.39285536
6	-3.24029217	-1.27224519	2.38285034
6	-3.96232625	-0.87477028	1.19924517
6	-3.84503276	-1.61937946	-0.01037470
6	-3.95510073	-0.88052779	-1.22419726
6	0.95020818	-3.32583939	2.40111076
6	-0.42033617	-3.43481050	2.39639172
6	-1.21957506	-2.46104466	3.08581014
6	1.72341847	-3.65569381	-1.19166648
6	1.06008141	-4.02189917	0.00996040
6	1.71624285	-3.64997147	1.21376727

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Vibrational frequencies

freq.	52.3	65.4	196.8	209.6	211.5	214.4
freq.	219.9	262.2	269.7	270.5	272.7	274.2
freq.	285.7	295.0	322.7	327.5	336.2	338.9
freq.	338.9	341.3	347.5	348.9	350.5	353.5
freq.	358.1	359.2	374.3	377.5	403.0	404.7
freq.	408.0	422.2	424.4	430.3	436.6	442.7
freq.	446.6	458.2	461.0	465.6	469.0	474.7
freq.	475.6	484.0	485.2	486.4	490.1	493.2
freq.	496.5	499.5	501.0	505.3	506.7	511.4
freq.	517.8	521.3	530.9	547.7	556.5	558.4
freq.	583.7	588.9	590.0	592.2	595.8	603.9
freq.	606.6	612.0	612.7	615.8	623.1	624.3
freq.	625.7	627.4	630.8	630.9	638.5	641.4
freq.	643.1	645.8	648.2	653.5	655.4	657.2
freq.	658.0	660.5	664.4	665.4	666.7	669.0
freq.	672.1	672.6	674.3	675.3	675.9	676.4
freq.	677.9	680.2	680.8	681.2	684.6	686.4
freq.	687.7	688.3	690.3	692.6	693.9	694.1

freq.	698.4	700.3	709.7	712.2	714.9	725.3
freq.	736.2	737.8	743.4	747.7	754.8	773.7
freq.	774.7	789.5	789.8	824.6	829.4	835.3
freq.	849.8	860.2	863.1	867.3	869.3	872.3
freq.	876.4	880.3	889.1	912.8	1005.3	1007.8
freq.	1010.6	1017.9	1018.2	1024.7	1026.9	1035.7
freq.	1038.6	1110.8	1117.4	1121.1	1124.0	1130.2
freq.	1140.3	1140.5	1146.3	1161.2	1164.0	1166.1
freq.	1181.5	1185.0	1192.0	1196.1	1205.1	1206.5
freq.	1215.2	1218.7	1222.2	1233.9	1235.3	1237.9
freq.	1246.5	1254.0	1260.3	1261.6	1267.4	1272.7
freq.	1273.1	1276.1	1277.6	1282.1	1287.6	1299.0
freq.	1315.6	1316.4	1318.5	1323.4	1324.1	1325.8
freq.	1328.3	1332.8	1338.7	1340.3	1341.3	1345.4
freq.	1352.2	1355.3	1364.2	1366.1	1368.5	1375.1
freq.	1378.7	1381.0	1382.8	1385.9	1390.6	1391.9
freq.	1391.9	1395.5	1412.3	1415.7	1420.0	1423.1
freq.	1424.8	1430.2	1433.1	1437.6	1437.7	1443.8
freq.	1448.1	1449.6	1455.0	1457.7	1466.5	1470.1
freq.	1475.2	1483.4	1486.7	1488.1	1496.6	1503.4
freq.	1503.5	1508.7	1521.5	1524.1	1525.9	1528.1
freq.	1529.3	1530.4	1532.4	1578.7	1588.9	1595.3
freq.	1596.1	1620.4	1626.7			

7. ===== Y@C₈₂ non-relativistic PBE/n3zv//PBE/n3zv

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Atomic Coordinates:

39	0.04791904	2.15378298	-0.00797041
6	3.84764132	1.18422605	-1.20880752
6	3.70326930	1.90420883	0.00376433
6	2.81294558	3.03207296	-0.00157229
6	3.84039346	1.18999789	1.22058438
6	4.03656868	-0.22792508	1.22266195
6	4.04570565	-0.97956639	0.01163851
6	4.04380548	-0.23368661	-1.20297741
6	3.05090843	1.54918283	2.38224145
6	2.14710050	2.63438490	2.34889100
6	2.07696494	3.43962251	1.15317181
6	0.95076734	2.51410158	3.09793128
6	2.82143036	-1.99693539	2.40950271
6	3.38383857	-0.73612253	2.40319858
6	2.71893454	0.33796047	3.08590299
6	1.44072672	0.14642405	3.68486974
6	0.60099126	1.29442024	3.75704358
6	2.88579538	-2.82372548	-1.19259762
6	3.45348193	-2.31942102	0.01305534
6	2.87860973	-2.81800025	1.21768413
6	-0.26557905	3.15755630	2.64524482
6	-0.33076622	4.00421855	1.48953854
6	0.90526452	4.19218852	0.73234637
6	-1.55097638	3.91884688	0.71774670
6	-1.36567893	2.32847694	3.08560027
6	-3.28324799	1.03533867	2.36534149
6	-2.56374582	2.25161923	2.32943453
6	-2.62504435	3.04749329	1.13867416
6	1.57854422	-2.23654538	3.09385511
6	0.81679498	-1.17428581	3.65882500
6	-0.64307967	-1.29115791	3.65373304
6	-1.47224362	-0.08729811	3.67554864
6	-0.82929656	1.18027238	3.74910852
6	-2.76173308	-0.10427386	3.06936580
6	-1.54660476	3.91539390	-0.75111290
6	-0.32181387	3.99718682	-1.51602320
6	0.90970228	4.18872240	-0.75236484
6	-0.24973886	3.14495498	-2.66723940
6	-2.61815804	3.04201286	-1.17428517
6	-3.26905467	1.02403033	-2.39527910
6	-2.54976497	2.24047624	-2.36085550
6	-1.34719798	2.31375742	-3.11020407
6	-4.00014256	0.55607501	1.19871560
6	-3.97766191	1.28786621	-0.01767589
6	-3.29779689	2.55098089	-0.01864994
6	-3.99290090	0.55030263	-1.23068826
6	0.96927879	2.49935996	-3.10960400
6	2.16113723	2.62323050	-2.35404299
6	2.08389096	3.43416026	-1.16261042

6	3.06510321	1.53788345	-2.37684534
6	0.62342657	1.27655138	-3.76498239
6	1.46270195	0.12891761	-3.68237183
6	2.73731430	0.32331983	-3.07670865
6	2.83573567	-2.00833261	-2.38862364
6	3.39811999	-0.74749688	-2.38495711
6	-1.20188643	-2.47640135	-3.08687206
6	-0.62127794	-1.30852539	-3.65683098
6	0.83860003	-1.19166237	-3.65377728
6	1.59695385	-2.25121393	-3.07923289
6	-0.80688029	1.16242233	-3.76503118
6	-2.74335761	-0.11891000	-3.09075444
6	-1.45027128	-0.10479654	-3.68929265
6	-1.11073965	-3.88425619	-1.19921267
6	-0.40622590	-3.44692516	-2.38821285
6	0.96438134	-3.33776034	-2.38511555
6	-1.11791120	-3.87854082	1.20550015
6	-0.40357934	-4.14081511	0.00588001
6	-3.22557391	-1.28312735	-2.40148172
6	-2.39928520	-3.24395103	1.20246742
6	-3.04138467	-2.84359351	-0.00506936
6	-2.39209988	-3.24967629	-1.20683825
6	-2.46753102	-2.43604557	-2.40227680
6	-2.48183252	-2.42464634	2.39355209
6	-3.23984108	-1.27176036	2.38276161
6	-3.96127624	-0.87420353	1.19933867
6	-3.84337531	-1.61844271	-0.01037120
6	-3.95404992	-0.87996264	-1.22428614
6	0.95010763	-3.32638596	2.40114983
6	-0.42049527	-3.43555563	2.39659007
6	-1.22029223	-2.46173112	3.08586719
6	1.72342757	-3.65677124	-1.19178219
6	1.06008765	-4.02295435	0.00996603
6	1.71625317	-3.65105293	1.21389454

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Vibrational frequencies

freq.	37.6	39.2	177.9	208.2	211.8	214.8
freq.	220.4	249.7	269.9	270.1	273.0	274.5
freq.	285.8	295.0	322.7	324.3	327.4	338.3
freq.	338.9	342.3	347.7	349.0	349.7	353.5
freq.	358.1	358.9	372.5	376.5	396.3	403.1
freq.	410.3	419.3	421.8	428.6	436.5	441.4
freq.	446.3	455.3	458.6	464.2	465.7	474.2
freq.	474.5	482.8	482.9	484.6	489.5	492.5
freq.	496.7	497.6	498.9	504.8	506.0	511.1
freq.	517.4	520.6	529.9	542.8	552.8	555.4
freq.	570.2	588.5	589.5	591.0	595.6	599.0
freq.	601.7	611.1	611.4	612.2	620.6	621.9
freq.	624.0	624.5	625.5	627.7	629.3	638.5
freq.	642.0	644.1	647.8	648.0	653.4	653.7
freq.	654.0	656.2	662.1	663.1	665.7	666.0
freq.	668.3	669.2	670.3	672.4	672.4	674.4
freq.	674.7	677.3	679.0	679.0	680.7	682.2

freq.	682.6	684.0	687.4	687.8	690.5	690.6
freq.	691.3	695.8	708.8	714.9	715.4	726.6
freq.	735.8	738.4	744.2	747.2	761.4	773.3
freq.	774.3	789.0	789.5	824.0	827.5	834.3
freq.	849.2	859.4	863.1	867.1	868.4	872.2
freq.	876.6	878.1	887.5	912.3	1003.5	1007.2
freq.	1009.2	1017.2	1017.9	1023.3	1026.7	1034.7
freq.	1037.6	1110.3	1117.0	1118.3	1123.7	1129.5
freq.	1139.0	1139.5	1144.8	1160.9	1163.4	1164.6
freq.	1181.3	1183.4	1190.7	1195.0	1203.2	1205.5
freq.	1214.5	1216.0	1221.1	1232.2	1233.3	1237.3
freq.	1245.9	1252.8	1259.8	1261.0	1267.3	1271.7
freq.	1273.0	1275.3	1276.6	1281.2	1285.8	1297.9
freq.	1312.8	1315.1	1317.6	1322.9	1323.0	1324.2
freq.	1326.2	1332.7	1338.7	1338.7	1339.1	1344.3
freq.	1351.1	1354.7	1362.4	1365.7	1367.5	1368.6
freq.	1375.0	1377.3	1378.7	1383.5	1388.9	1390.0
freq.	1391.2	1393.7	1410.9	1412.8	1417.7	1421.2
freq.	1422.9	1429.3	1430.7	1436.4	1437.2	1440.7
freq.	1445.0	1447.3	1452.3	1456.6	1464.5	1467.2
freq.	1473.3	1482.1	1485.2	1486.6	1495.8	1501.6
freq.	1501.9	1506.3	1520.4	1523.8	1524.3	1526.5
freq.	1527.9	1529.3	1530.5	1576.7	1587.3	1592.2
freq.	1593.6	1619.0	1625.5			
