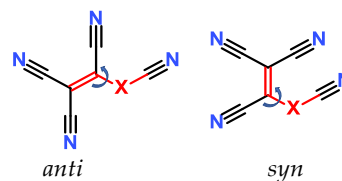
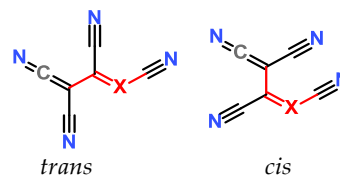


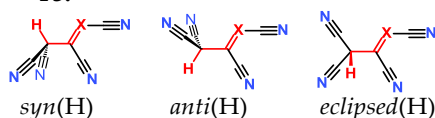
Anion, T1, T2, T6:



T3, T4, T5:



T3:



		GEO file	FR file	Folder	Cosmo file In CN_Cosmo folder
1					
Anion	BP86/def-TZVP BP86/def2-TZVPP BP86/def2-TZVPPD B3LYP/def2-TZVPPD B3LYP/6-311+G(d,p) G4(MP2) W1RO CBS-APNO	job_GEO_238 job_GEO_491 job_GEO_715 job_GEO_719 JOB_1000 JOB_1000_1 JOB_1000_2 JOB_1000_3	job_SP_239 job_SP_497 job_SP_717 job_SP_723	CN_2 CN_1 CN_1 CN_1 CN_GAU CN_GAU CN_GAU CN_GAU	COSMO-BP-TZVPD-FINE_17
Neutral					
T1	BP86/def-TZVP BP86/def-TZVP BP86/def2-TZVPP BP86/def2-TZVPPD B3LYP/def2-TZVPPD B3LYP/6-311+G(d,p) G4(MP2) W1RO CBS-APNO	job_GEO_242 job_GEO_361 job_GEO_492 job_GEO_716 job_GEO_720 JOB_1001 JOB_1001_1 JOB_1001_2 JOB_1001_3	job_SP_243 job_SP_362 job_SP_498 job_SP_718 job_SP_724	CN_2 CN_2 CN_1 CN_1 CN_1 CN_GAU CN_GAU CN_GAU CN_GAU	COSMO-BP-TZVPD-FINE_19
T2					
2					
Anion	BP86/def-TZVP BP86/def2-TZVPP BP86/def2-TZVPPD B3LYP/def2-TZVPPD B3LYP/6-311+G(d,p) G4(MP2) W1RO CBS-APNO	job_GEO_223 job_GEO_501 job_GEO_725 job_GEO_727 JOB_1002 JOB_1002_1 JOB_1002_2 JOB_1002_3	job_SP_231 job_SP_503 job_SP_729 job_SP_731	CN_2 CN_1 CN_1 CN_1 CN_GAU CN_GAU CN_GAU CN_GAU	COSMO-BP-TZVPD-FINE_21
Neutral					
T1	BP86/def-TZVP BP86/def2-TZVPP BP86/def2-TZVPPD B3LYP/def2-TZVPPD B3LYP/6-311+G(d,p) G4(MP2) W1RO CBS-APNO	job_GEO_224 job_GEO_502 job_GEO_726 job_GEO_728 JOB_1003 JOB_1003_1 JOB_1003_2 JOB_1003_3	job_SP_232 job_SP_505 job_SP_730 job_SP_732	CN_2 CN_1 CN_1 CN_1 CN_GAU CN_GAU CN_GAU CN_GAU	COSMO-BP-TZVPD-FINE_23
T3; eclipsed(H)	BP86/def-TZVP	job_GEO_225	job_SP_233	CN_2	
T3; syn(H)	BP86/def-TZVP	job_GEO_78	job_SP_80	CN_1	
T3; anti(H)	BP86/def-TZVP	job_GEO_82	job_SP_83	CN_1	
T4	BP86/def-TZVP	job_GEO_32	job_SP_34	CN_1	COSMO-BP-TZVPD-FINE_316
T5	BP86/def-TZVP	job_GEO_226	job_SP_234	CN_2	COSMO-BP-TZVPD-FINE_314
T6	BP86/def-TZVP	job_GEO_33	job_SP_35	CN_1	

3					
Anion	BP86/def-TZVP BP86/def2-TZVPP BP86/def2-TZVPPD B3LYP/def2-TZVPPD B3LYP/6-311+G(d,p) G4(MP2) W1RO CBS-APNO	job_GEO_363 job_GEO_506 job_GEO_733 job_GEO_734 JOB_1004 JOB_1004_1 JOB_1004_2 JOB_1004_3	job_SP_364 job_SP_508 job_SP_760 job_SP_761	CN_2 CN_1 CN_1 CN_1 CN_GAU CN_GAU CN_GAU CN_GAU	COSMO-BP-TZVPD-FINE_26
Neutral					
T1	BP86/def-TZVP	job_GEO_247	job_SP_250	CN_2	
T2	BP86/def-TZVP BP86/def2-TZVPP BP86/def2-TZVPPD B3LYP/def2-TZVPPD B3LYP/6-311+G(d,p) G4(MP2) W1RO CBS-APNO	job_GEO_248 job_GEO_507 job_GEO_735 job_GEO_736 JOB_1005 JOB_1005_1 JOB_1005_2 JOB_1005_3	job_SP_251 job_SP_509 job_SP_762 job_SP_763	CN_2 CN_1 CN_1 CN_1 CN_GAU CN_GAU CN_GAU CN_GAU	COSMO-BP-TZVPD-FINE_28
4					
Anion					
anti	BP86/def-TZVP BP86/def2-TZVPP BP86/def2-TZVPPD B3LYP/def2-TZVPPD B3LYP/6-311+G(d,p) G4(MP2) W1RO CBS-APNO	job_GEO_254 job_GEO_510 job_GEO_737 job_GEO_738 JOB_1006 JOB_1006_1 JOB_1006_2 JOB_1006_3	job_SP_263 job_SP_515 job_SP_776 job_SP_777	CN_2 CN_1 CN_1 CN_1 CN_GAU CN_GAU CN_GAU CN_GAU	COSMO-BP-TZVPD-FINE_116
syn	BP86/def-TZVP BP86/def2-TZVPP	job_GEO_332 job_GEO_511	job_SP_340 job_SP_516	CN_2 CN_1	COSMO-BP-TZVPD-FINE_30
Neutral					
T1; syn	BP86/def-TZVP	job_GEO_255	job_SP_264	CN_2	
T1; anti	BP86/def-TZVP	job_GEO_333	job_SP_341	CN_2	
T2; anti	BP86/def-TZVP BP86/def2-TZVPP BP86/def2-TZVPPD B3LYP/def2-TZVPPD B3LYP/6-311+G(d,p) G4(MP2) W1RO CBS-APNO	job_GEO_258 job_GEO_514 job_GEO_739 job_GEO_740 JOB_1007 JOB_1007_1 JOB_1007_2 JOB_1007_3	job_SP_267 job_SP_518 job_SP_778 job_SP_779	CN_2 CN_1 CN_1 CN_1 CN_GAU CN_GAU CN_GAU CN_GAU	COSMO-BP-TZVPD-FINE_118
T2; syn	BP86/def-TZVP BP86/def2-TZVPP	job_GEO_335 job_GEO_513	job_SP_343 job_SP_517	CN_2 CN_1	COSMO-BP-TZVPD-FINE_32
T3; trans, eclipsed(H)	BP86/def-TZVP	job_GEO_256	job_SP_265	CN_2	
T3; trans, syn(H)	BP86/def-TZVP	job_GEO_85	job_SP_95	CN_1	
T3; cis, anti(H)	BP86/def-TZVP	job_GEO_22	job_SP_23	CN_1	
T3; cis, syn(H)	BP86/def-TZVP	job_GEO_84	job_SP_94	CN_1	
T4; trans	BP86/def-TZVP	job_GEO_257	job_SP_266	CN_2	
T4; cis	BP86/def-TZVP	job_GEO_334	job_SP_342	CN_2	
T5; trans	BP86/def-TZVP	job_GEO_37	job_SP_45	CN_1	
T5; cis	BP86/def-TZVP	job_GEO_38	job_SP_42	CN_1	
T6; anti	BP86/def-TZVP	job_GEO_40	job_SP_44	CN_1	
T6; syn	BP86/def-TZVP	job_GEO_39	job_SP_43	CN_1	
5					
Anion					
Anion; anti-syn (syn facing forward)	BP86/def-TZVP	job_GEO_259	job_SP_269	CN_2	
Anion; anti-syn (syn facing backward)	BP86/def-TZVP	job_GEO_471	job_SP_475	CN_1	COSMO-BP-TZVPD-FINE_120
anti-anti	BP86/def2-TZVPP BP86/def-TZVP BP86/def2-TZVPP BP86/def2-TZVPPD B3LYP/def2-TZVPPD B3LYP/6-311+G(d,p) G4(MP2) CBS-APNO	job_GEO_522 job_GEO_19 job_GEO_741 job_GEO_742 job_GEO_775 JOB_1008 JOB_1008_1 JOB_1008_3	job_SP_524 job_SP_20 job_SP_770 job_SP_771 job_SP_794	CN_1 CN_1 CN_1 CN_1 CN_1 CN_GAU CN_GAU CN_GAU	COSMO-BP-TZVPD-FINE_53 COSMO-BP-TZVPD-FINE_122
syn-syn	BP86/def-TZVP	job_GEO_25	job_SP_26	CN_1	COSMO-BP-TZVPD-FINE_124
Neutral					
T1; anti-syn (syn facing forward)	BP86/def-TZVP	job_GEO_472	job_SP_476	CN_1	COSMO-BP-TZVPD-FINE_126
T1; anti-syn (syn facing backward)	BP86/def-TZVP BP86/def2-TZVPP BP86/def-TZVP	job_GEO_260 job_GEO_523 job_GEO_27	job_SP_270 job_SP_525 job_SP_29	CN_2 CN_1 CN_1	COSMO-BP-TZVPD-FINE_55 COSMO-BP-TZVPD-FINE_128
T1; syn-syn	BP86/def-TZVP	job_GEO_795	job_SP_812	CN_1	COSMO-BP-TZVPD-FINE_130
T1; anti-anti	BP86/def2-TZVPP BP86/def2-TZVPPD B3LYP/def2-TZVPPD B3LYP/6-311+G(d,p) G4(MP2) CBS-APNO	job_GEO_744 job_GEO_745 job_GEO_758 JOB_1009 JOB_1009_1 JOB_1009_3	job_SP_773 job_SP_774 job_SP_772	CN_1 CN_1 CN_1 CN_GAU CN_GAU CN_GAU	
T3; cis-anti, eclipsed(H)	BP86/def-TZVP	job_GEO_261	job_SP_271	CN_2	
T3; cis-anti, syn(H)	BP86/def-TZVP	job_GEO_91	job_SP_104	CN_1	
T3; trans-anti, syn(H)	BP86/def-TZVP	job_GEO_338	job_SP_349	CN_2	
T3; trans-anti, eclipsed(H)	BP86/def-TZVP	job_GEO_96	job_SP_105	CN_1	
T3; cis-syn, eclipsed(H)	BP86/def-TZVP	job_GEO_75	job_SP_106	CN_1	
T3; cis-syn, syn(H)	BP86/def-TZVP	job_GEO_92	job_SP_107	CN_1	
T3; trans-syn, syn(H)	BP86/def-TZVP	job_GEO_67	job_SP_76	CN_1	
T3; trans-syn, eclipsed(H)	BP86/def-TZVP	job_GEO_93	job_SP_108	CN_1	
T4; cis-anti	BP86/def-TZVP	job_GEO_262	job_SP_272	CN_2	
T4; trans-anti	BP86/def-TZVP	job_GEO_339	job_SP_347	CN_2	
T4; cis-syn	BP86/def-TZVP	job_GEO_51	job_SP_72	CN_1	
T4; trans-syn	BP86/def-TZVP	job_GEO_47	job_SP_59	CN_1	

T5; trans-anti	BP86/def-TZVP	job_GEO_48	job_SP_64	CN_1	
T5; cis-syn	BP86/def-TZVP	job_GEO_49	job_SP_65	CN_1	
T5; trans-syn	BP86/def-TZVP	job_GEO_50	job_SP_57	CN_1	
T5; cis-anti	BP86/def-TZVP	job_GEO_905	job_SP_906	CN_1	
T6; anti-anti	BP86/def-TZVP	job_GEO_60	job_SP_68	CN_1	
T6; syn-syn	BP86/def-TZVP	job_GEO_61	job_SP_73	CN_1	
T6; anti-syn	BP86/def-TZVP	job_GEO_62	job_SP_70	CN_1	
T6; syn-anti	BP86/def-TZVP	job_GEO_63	job_SP_74	CN_1	
6					
Anion					
	BP86/def-TZVP	job_GEO_273	job_SP_290	CN_2	
	BP86/def2-TZVPP	job_GEO_538	job_SP_540	CN_1	COSMO-BP-TZVPD-FINE_38
	BP86/def2-TZVPPD	job_GEO_747	job_SP_799	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_748	job_SP_800	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1010		CN_GAU	
	G4(MP2)	JOB_1010_1		CN_GAU	
	W1RO	JOB_1010_2		CN_GAU	
	CBS-APNO	JOB_1010_3		CN_GAU	
Neutral					
T1	BP86/def-TZVP	job_GEO_274	job_SP_291	CN_2	
T2	BP86/def-TZVP	job_GEO_275	job_SP_292	CN_2	
	BP86/def2-TZVPP	job_GEO_539	job_SP_542	CN_1	COSMO-BP-TZVPD-FINE_40
	BP86/def2-TZVPPD	job_GEO_749	job_SP_801	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_750	job_SP_802	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1011		CN_GAU	
	G4(MP2)	JOB_1011_1		CN_GAU	
	W1RO	JOB_1011_2		CN_GAU	
	CBS-APNO	JOB_1011_3		CN_GAU	
7					
Anion					
	BP86/def-TZVP	job_GEO_276	job_SP_293	CN_2	
	BP86/def2-TZVPP	job_GEO_544	job_SP_570	CN_1	COSMO-BP-TZVPD-FINE_57
	BP86/def2-TZVPPD	job_GEO_751	job_SP_803	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_752	job_SP_804	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1012		CN_GAU	
	G4(MP2)	JOB_1012_1		CN_GAU	
	W1RO	JOB_1012_2		CN_GAU	
	CBS-APNO	JOB_1012_3		CN_GAU	
Neutral					
T3 = T1; anti(H)	BP86/def-TZVP	job_GEO_277	job_SP_296	CN_2	
T3 = T1; syn(H)	BP86/def-TZVP	job_GEO_307	job_SP_309	CN_2	
T2 = T4	BP86/def-TZVP	job_GEO_278	job_SP_295	CN_2	
T2 = T5	BP86/def-TZVP	job_GEO_109	job_SP_113	CN_1	
	BP86/def2-TZVPP	job_GEO_543	job_SP_571	CN_1	COSMO-BP-TZVPD-FINE_71
	BP86/def2-TZVPPD	job_GEO_753	job_SP_805	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_754	job_SP_806	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1013		CN_GAU	
	G4(MP2)	JOB_1013_1		CN_GAU	
	W1RO	JOB_1013_2		CN_GAU	
	CBS-APNO	JOB_1013_3		CN_GAU	
T6	BP86/def-TZVP	job_GEO_110	job_SP_112	CN_1	
8					
Anion					
syn-syn	BP86/def-TZVP	job_GEO_279	job_SP_297	CN_2	COSMO-BP-TZVPD-FINE_132
anti-syn	BP86/def-TZVP	job_GEO_308	job_SP_316	CN_2	COSMO-BP-TZVPD-FINE_134
	BP86/def2-TZVPP	job_GEO_755	job_SP_807	CN_1	
	BP86/def2-TZVPPD	job_GEO_756	job_SP_808	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_757	job_SP_809	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1014		CN_GAU	
	G4(MP2)	JOB_1014_1		CN_GAU	
	CBS-APNO	JOB_1014_3		CN_GAU	
anti-anti	BP86/def-TZVP	job_GEO_116	job_SP_117	CN_1	
	BP86/def2-TZVPP	job_GEO_545	job_SP_572	CN_1	COSMO-BP-TZVPD-FINE_73
Neutral					
T1; syn-syn	BP86/def-TZVP	job_GEO_175	job_SP_184	CN_1	
T1; anti-anti	BP86/def-TZVP	job_GEO_114	job_SP_118	CN_1	
T1; anti-syn = syn-anti	BP86/def-TZVP	job_GEO_280	job_SP_298	CN_2	
T2; anti-anti	BP86/def-TZVP	job_GEO_283	job_SP_301	CN_2	
	BP86/def2-TZVPP	job_GEO_546	job_SP_573	CN_1	COSMO-BP-TZVPD-FINE_114
T2; syn-anti	BP86/def-TZVP	job_GEO_317	job_SP_322	CN_2	COSMO-BP-TZVPD-FINE_136
	BP86/def2-TZVPP	job_GEO_810	job_SP_811	CN_1	
	BP86/def2-TZVPPD	job_GEO_823	job_SP_826	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_824	job_SP_835	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1015		CN_GAU	
	G4(MP2)	JOB_1015_1		CN_GAU	
	CBS-APNO	JOB_1015_3		CN_GAU	
T2; syn-syn	BP86/def-TZVP	job_GEO_123	job_SP_124	CN_1	COSMO-BP-TZVPD-FINE_138
T3; cis-anti, anti(H)	BP86/def-TZVP	job_GEO_315	job_SP_321	CN_2	
T3; cis-anti, syn(H)	BP86/def-TZVP	job_GEO_152	job_SP_153	CN_1	
T3; cis-anti, eclipsed(H)	BP86/def-TZVP	job_GEO_170	job_SP_171	CN_1	
T3; trans-anti, syn(H)	BP86/def-TZVP	job_GEO_154	job_SP_155	CN_1	
T3; trans-anti, anti(H)	BP86/def-TZVP	job_GEO_162	job_SP_174	CN_1	
T3; cis-syn, eclipsed(H)	BP86/def-TZVP	job_GEO_157	job_SP_167	CN_1	
T3; trans-syn, syn(H)	BP86/def-TZVP	job_GEO_159	job_SP_168	CN_1	
T3; trans-syn, anti(H)	BP86/def-TZVP	job_GEO_161	job_SP_173	CN_1	
T4; cis-anti	BP86/def-TZVP	job_GEO_122	job_SP_125	CN_1	
T4; cis-syn	BP86/def-TZVP	job_GEO_121	job_SP_126	CN_1	
T4; trans-syn	BP86/def-TZVP	job_GEO_127	job_SP_128	CN_1	
T4; trans-anti	BP86/def-TZVP	job_GEO_289	job_SP_300	CN_2	
T5; trans-anti	BP86/def-TZVP	job_GEO_129	job_SP_133	CN_1	
T5; cis-syn	BP86/def-TZVP	job_GEO_130	job_SP_134	CN_1	

T5; cis-anti	BP86/def-TZVP	job_GEO_131	job_SP_135	CN_1	
T5; trans-syn	BP86/def-TZVP	job_GEO_132	job_SP_136	CN_1	
T6; anti-anti	BP86/def-TZVP	job_GEO_137	job_SP_142	CN_1	
T6; anti-syn	BP86/def-TZVP	job_GEO_150	job_SP_151	CN_1	
T6; syn-anti	BP86/def-TZVP	job_GEO_141	job_SP_147	CN_1	
T6; syn-syn	BP86/def-TZVP	job_GEO_140	job_SP_149	CN_1	
9					
Anion					
symmetrical					
	BP86/def-TZVP	job_GEO_285	job_SP_302	CN_2	
	BP86/def2-TZVPP	job_GEO_549	job_SP_574	CN_1	COSMO-BP-TZVPD-FINE_63
	BP86/def2-TZVPPD	job_GEO_837	job_SP_841	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_838	job_SP_845	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1016		CN_GAU	
	G4(MP2)	JOB_1016_1		CN_GAU	
asymmetrical					
	BP86/def-TZVP	job_GEO_327	job_SP_331	CN_2	
	BP86/def2-TZVPP	job_GEO_550	job_SP_575	CN_1	COSMO-BP-TZVPD-FINE_65
Neutral					
T1; asymmetrical, anti-syn-syn; H facing backward	BP86/def-TZVP	job_GEO_286	job_SP_303	CN_2	COSMO-BP-TZVPD-FINE_306
T1; symmetrical, syn-syn-syn; H facing backward	BP86/def-TZVP	job_GEO_324	job_SP_328	CN_2	COSMO-BP-TZVPD-FINE_308
T1; symmetrical, anti-anti-anti; H facing backward	BP86/def-TZVP	job_GEO_178	job_SP_182	CN_1	
	BP86/def2-TZVPP	job_GEO_547	job_SP_576	CN_1	
	BP86/def2-TZVPPD	job_GEO_869	job_SP_871	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_840	job_SP_846	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1017		CN_GAU	
	G4(MP2)	JOB_1017_1		CN_GAU	
T1; asymmetrical, anti-anti-syn; H facing backward	BP86/def-TZVP	job_GEO_177	job_SP_181	CN_1	COSMO-BP-TZVPD-FINE_310
T3; trans-syn-syn, eclipsed(H)	BP86/def-TZVP	job_GEO_287	job_SP_306	CN_2	
T3; trans-syn-syn, anti(H)	BP86/def-TZVP	job_GEO_325	job_SP_329	CN_2	
T3; trans-syn-syn, syn(H)	BP86/def-TZVP	job_GEO_209	job_SP_210	CN_1	
T3; trans-syn-anti, syn(H)	BP86/def-TZVP	job_GEO_211	job_SP_233	CN_1	
T3; trans-syn-anti, anti(H)	BP86/def-TZVP	job_GEO_212	job_SP_223	CN_1	
T3; trans-syn-anti, eclipsed(H)	BP86/def-TZVP	job_GEO_213	job_SP_225	CN_1	
T3; trans-anti-anti, syn(H)	BP86/def-TZVP	job_GEO_220	job_SP_226	CN_1	
T3; trans-anti-anti, anti(H)	BP86/def-TZVP	job_GEO_221	job_SP_234	CN_1	
T3; trans-anti-anti, syn(H) (symmetrical)	BP86/def-TZVP	job_GEO_216	job_SP_228	CN_1	
T3; trans-syn-anti, syn(H)	BP86/def-TZVP	job_GEO_217	job_SP_229	CN_1	
T3; trans-syn-anti, anti(H)	BP86/def-TZVP	job_GEO_218	job_SP_235	CN_1	
T3; trans-syn-anti, eclipsed(H)	BP86/def-TZVP	job_GEO_231	job_SP_232	CN_1	
T4; trans-anti-syn	BP86/def-TZVP	job_GEO_288	job_SP_304	CN_2	COSMO-BP-TZVPD-FINE_140
T4; trans-syn-anti	BP86/def-TZVP	job_GEO_179	job_SP_187	CN_1	
T4; trans-syn-anti	BP86/def2-TZVPP	job_GEO_548	job_SP_577	CN_1	COSMO-BP-TZVPD-FINE_69
T4; trans-syn-syn	BP86/def-TZVP	job_GEO_185	job_SP_189	CN_1	COSMO-BP-TZVPD-FINE_142
T4; trans-anti-anti (symmetrical)	BP86/def-TZVP	job_GEO_183	job_SP_186	CN_1	COSMO-BP-TZVPD-FINE_144
T5; trans-anti-syn	BP86/def-TZVP	job_GEO_193	job_SP_198	CN_1	
T5; trans-syn-anti	BP86/def-TZVP	job_GEO_190	job_SP_199	CN_1	
T5; trans-syn-syn	BP86/def-TZVP	job_GEO_192	job_SP_200	CN_1	
T5; trans-anti-anti (symmetrical)	BP86/def-TZVP	job_GEO_191	job_SP_207	CN_1	
T6; anti-anti-syn	BP86/def-TZVP	job_GEO_197	job_SP_202	CN_1	
T6; anti-syn-anti	BP86/def-TZVP	job_GEO_194	job_SP_203	CN_1	
T6; anti-syn-syn	BP86/def-TZVP	job_GEO_196	job_SP_206	CN_1	
T6; anti-anti-anti (symmetrical)	BP86/def-TZVP	job_GEO_195	job_SP_208	CN_1	
10					
Anion					
Pyramidal					
	BP86/def-TZVP	job_GEO_365	job_SP_366	CN_2	
	BP86/def2-TZVPP	job_GEO_551	job_SP_578	CN_1	COSMO-BP-TZVPD-FINE_75
	BP86/def2-TZVPPD	job_GEO_847	job_SP_872	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_848	job_SP_873	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1018		CN_GAU	
	G4(MP2)	JOB_1018_1		CN_GAU	
	W1RO	JOB_1018_2		CN_GAU	
	CBS-APNO	JOB_1018_3		CN_GAU	
Neutral					
T2					
	BP86/def-TZVP	job_GEO_352	job_SP_355	CN_2	
	BP86/def2-TZVPP	job_GEO_552	job_SP_579	CN_1	COSMO-BP-TZVPD-FINE_77
	BP86/def2-TZVPPD	job_GEO_849	job_SP_874	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_850	job_SP_875	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1019		CN_GAU	
	G4(MP2)	JOB_1019_1		CN_GAU	
	W1RO	JOB_1019_2		CN_GAU	
	CBS-APNO	JOB_1019_3		CN_GAU	
11					
Anion					
	BP86/def-TZVP	job_GEO_356	job_SP_390	CN_2	
	BP86/def2-TZVPP	job_GEO_553	job_SP_598	CN_1	COSMO-BP-TZVPD-FINE_79
	BP86/def2-TZVPPD	job_GEO_851	job_SP_878	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_852	job_SP_879	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1020		CN_GAU	
	G4(MP2)	JOB_1020_1		CN_GAU	
	W1RO	JOB_1020_2		CN_GAU	
	CBS-APNO	JOB_1020_3		CN_GAU	
T2; protonated on CN-1	BP86/def-TZVP	job_GEO_360	job_SP_392	CN_2	
T2; protonated on CN-2	BP86/def-TZVP	job_GEO_238	job_SP_242	CN_1	
T2; protonated on CN-3	BP86/def-TZVP	job_GEO_239	job_SP_243	CN_1	
	BP86/def2-TZVPP	job_GEO_554	job_SP_599	CN_1	COSMO-BP-TZVPD-FINE_81
	BP86/def2-TZVPPD	job_GEO_853	job_SP_880	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_854	job_SP_881	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1021		CN_GAU	
	G4(MP2)	JOB_1021_1		CN_GAU	
	W1RO	JOB_1021_2		CN_GAU	
	CBS-APNO	JOB_1021_3		CN_GAU	
T4	BP86/def-TZVP	job_GEO_244	job_SP_245	CN_1	

T5	BP86/def-TZVP	job_GEO_389	job_SP_391	CN_1	
T6	BP86/def-TZVP	job_GEO_237	job_SP_241	CN_1	

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Conformer name the way CN or HCN group facing away.

Part of the name in () indicates that the group weakly exhibits this conformation and is on the same plane of the formed plane.

Anion					
anti-syn; asymmetric	BP86/def-TZVP	job_GEO_454	job_SP_457	CN_2	
	BP86/def2-TZVPP	job_GEO_555	job_SP_600	CN_1	COSMO-BP-TZVPD-FINE_83
	BP86/def2-TZVPPD	job_GEO_855	job_SP_882	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_856	job_SP_883	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1022		CN_GAU	
	G4(MP2)	JOB_1022_1		CN_GAU	
	CBS-APNO	JOB_1022_3		CN_GAU	
syn-syn; symmetric	BP86/def-TZVP	job_GEO_455	job_SP_458	CN_2	COSMO-BP-TZVPD-FINE_147
anti-anti; symmetric	BP86/def-TZVP	job_GEO_456	job_SP_459	CN_2	COSMO-BP-TZVPD-FINE_149
Neutral					
T2; protonated on CN-1; anti-syn	BP86/def-TZVP	job_GEO_114	job_SP_115	CN_3	
	BP86/def2-TZVPP	job_GEO_556	job_SP_601	CN_1	COSMO-BP-TZVPD-FINE_85
	BP86/def2-TZVPPD	job_GEO_857	job_SP_884	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_858	job_SP_885	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1023		CN_GAU	
	G4(MP2)	JOB_1023_1		CN_GAU	
	CBS-APNO	JOB_1023_3		CN_GAU	
T2; protonated on CN-1; syn-syn	BP86/def-TZVP	job_GEO_253	job_SP_304	CN_1	COSMO-BP-TZVPD-FINE_151
T2; protonated on CN-1; rather anti-syn	BP86/def-TZVP	job_GEO_252	job_SP_305	CN_1	COSMO-BP-TZVPD-FINE_167
T2; protonated on CN-2; syn-syn	BP86/def-TZVP	job_GEO_255	job_SP_306	CN_1	
T2; protonated on CN-2; anti-syn	BP86/def-TZVP	job_GEO_250	job_SP_307	CN_1	
T2; protonated on CN-2; syn-anti	BP86/def-TZVP	job_GEO_251	job_SP_308	CN_1	
T2; protonated on CN-2; anti-anti	BP86/def-TZVP	job_GEO_254	job_SP_309	CN_1	COSMO-BP-TZVPD-FINE_169
T4; cis-anti	BP86/def-TZVP	job_GEO_113	job_SP_116	CN_3	
T4; cis-syn	BP86/def-TZVP	job_GEO_258	job_SP_267	CN_1	
T4; trans-anti	BP86/def-TZVP	job_GEO_256	job_SP_295	CN_1	
T4; trans-syn	BP86/def-TZVP	job_GEO_257	job_SP_296	CN_1	
T5; cis-anti	BP86/def-TZVP	job_GEO_261	job_SP_297	CN_1	
T5; cis-syn	BP86/def-TZVP	job_GEO_262	job_SP_283	CN_1	
T5; trans-syn	BP86/def-TZVP	job_GEO_286	job_SP_298	CN_1	
T5; trans-anti	BP86/def-TZVP	job_GEO_259	job_SP_299	CN_1	
T6; anti-syn	BP86/def-TZVP	job_GEO_260	job_SP_300	CN_1	
T6; syn-syn	BP86/def-TZVP	job_GEO_264	job_SP_301	CN_1	
T6; anti-anti	BP86/def-TZVP	job_GEO_266	job_SP_302	CN_1	
T6; syn-anti	BP86/def-TZVP	job_GEO_268	job_SP_281	CN_1	
	BP86/def-TZVP	job_GEO_265	job_SP_281	CN_1	

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Anion					
anti-syn-anti	BP86/def-TZVP	job_GEO_129	job_SP_136	CN_3	COSMO-BP-TZVPD-FINE_155
anti-syn-syn	BP86/def-TZVP	job_GEO_131	job_SP_138	CN_3	COSMO-BP-TZVPD-FINE_157
syn-syn-syn	BP86/def-TZVP	job_GEO_248	job_SP_249	CN_1	COSMO-BP-TZVPD-FINE_153
anti-anti-anti	BP86/def-TZVP	job_GEO_137	job_SP_139	CN_3	
	BP86/def2-TZVPP	job_GEO_557	job_SP_604	CN_1	COSMO-BP-TZVPD-FINE_87
	BP86/def2-TZVPPD	job_GEO_859	job_SP_886	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_860	job_SP_887	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1024		CN_GAU	
	G4(MP2)	JOB_1024_1		CN_GAU	
Neutral					
T2, anti-anti-syn	BP86/def-TZVP	job_GEO_127	job_SP_134	CN_3	COSMO-BP-TZVPD-FINE_159
T2, anti-anti-anti	BP86/def-TZVP	job_GEO_100	job_SP_106	CN_3	COSMO-BP-TZVPD-FINE_161
	BP86/def2-TZVPP	job_GEO_558	job_SP_603	CN_1	COSMO-BP-TZVPD-FINE_89
	BP86/def2-TZVPPD	job_GEO_861	job_SP_888	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_862	job_SP_889	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1025		CN_GAU	
	G4(MP2)	JOB_1025_1		CN_GAU	
T2, anti-syn-syn	BP86/def-TZVP	job_GEO_313	job_SP_314	CN_1	COSMO-BP-TZVPD-FINE_163
T2, syn-syn-syn	BP86/def-TZVP	job_GEO_312	job_SP_315	CN_1	COSMO-BP-TZVPD-FINE_165
T4, trans-syn-anti	BP86/def-TZVP	job_GEO_128	job_SP_135	CN_3	
T4; cis-syn-anti	BP86/def-TZVP	job_GEO_317	job_SP_366	CN_1	
T4; trans-syn-syn	BP86/def-TZVP	job_GEO_318	job_SP_367	CN_1	
T4; cis-syn-syn (symmetrical)	BP86/def-TZVP	job_GEO_319	job_SP_373	CN_1	
T4; trans-anti-anti (symmetrical)	BP86/def-TZVP	job_GEO_320	job_SP_374	CN_1	
T4; cis-anti-anti	BP86/def-TZVP	job_GEO_321	job_SP_375	CN_1	
T4; trans-anti-syn	BP86/def-TZVP	job_GEO_322	job_SP_371	CN_1	
T4; cis-anti-syn	BP86/def-TZVP	job_GEO_323	job_SP_372	CN_1	
T5; trans-(anti)-anti	BP86/def-TZVP	job_GEO_340	job_SP_377	CN_1	
T5; cis-syn-anti	BP86/def-TZVP	job_GEO_333	job_SP_378	CN_1	
T5; trans-(anti)-syn	BP86/def-TZVP	job_GEO_334	job_SP_383	CN_1	
T5; cis-syn-(syn)	BP86/def-TZVP	job_GEO_343	job_SP_380	CN_1	
T5; trans-anti-anti	BP86/def-TZVP	job_GEO_336	job_SP_381	CN_1	
T5; cis-anti-anti	BP86/def-TZVP	job_GEO_337	job_SP_382	CN_1	
T5; trans-anti-syn	BP86/def-TZVP	job_GEO_338	job_SP_392	CN_1	
T5; cis-anti-(anti)	BP86/def-TZVP	job_GEO_347	job_SP_385	CN_1	
T6; trans-syn-anti	BP86/def-TZVP	job_GEO_348	job_SP_402	CN_1	
T6; cis-(anti)-anti	BP86/def-TZVP	job_GEO_341	job_SP_394	CN_1	
T6; trans-syn-(syn)	BP86/def-TZVP	job_GEO_342	job_SP_403	CN_1	
T6; cis-syn-syn (symmetrical)	BP86/def-TZVP	job_GEO_335	job_SP_401	CN_1	
T6; trans-anti-anti (symmetrical)	BP86/def-TZVP	job_GEO_344	job_SP_404	CN_1	
T6; cis-anti-anti	BP86/def-TZVP	job_GEO_345	job_SP_398	CN_1	
T6; trans-anti-(anti)	BP86/def-TZVP	job_GEO_346	job_SP_405	CN_1	
T6; cis-anti-syn	BP86/def-TZVP	job_GEO_339	job_SP_400	CN_1	

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Anion

conformer I	BP86/def-TZVP	job_GEO_86	job_SP_88	CN_3	COSMO-BP-TZVPD-FINE_175
conformer II	BP86/def-TZVP	job_GEO_406	job_SP_421	CN_1	
	BP86/def2-TZVPP	job_GEO_559	job_SP_595	CN_1	COSMO-BP-TZVPD-FINE_91
conformer III; most stable from CosmoConf	BP86/def-TZVP	job_GEO_675	job_SP_676	CN_1	COSMO-BP-TZVPD-FINE_171
	BP86/def2-TZVPP	job_GEO_863	job_SP_890	CN_1	
	BP86/def2-TZVPPD	job_GEO_864	job_SP_891	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1026		CN_GAU	
	G4(MP2)	JOB_1026_1		CN_GAU	
conformer IV	BP86/def-TZVP	job_GEO_677	job_SP_680	CN_1	COSMO-BP-TZVPD-FINE_173
Neutral					
T4; conformer I	BP86/def-TZVP	job_GEO_109	job_SP_117	CN_3	
T4; conformer I	BP86/def-TZVP	job_GEO_437	job_SP_449	CN_1	
T4; conformer I	BP86/def-TZVP	job_GEO_440	job_SP_450	CN_1	
T4; conformer I	BP86/def-TZVP	job_GEO_443	job_SP_451	CN_1	
T4; conformer I	BP86/def-TZVP	job_GEO_446	job_SP_452	CN_1	
T4; conformer II	BP86/def-TZVP	job_GEO_410	job_SP_424	CN_1	
T4; conformer II	BP86/def-TZVP	job_GEO_422	job_SP_433	CN_1	
T4; conformer II	BP86/def-TZVP	job_GEO_416	job_SP_429	CN_1	
T4; conformer II	BP86/def-TZVP	job_GEO_419	job_SP_434	CN_1	
T4; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T4_1)	job_SP_685	CN_1	
T4; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T4_2)	job_SP_686	CN_1	
T4; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T4_3)	job_SP_687	CN_1	
T4; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T4_4)	job_SP_688	CN_1	
T4; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T4_1)	job_SP_698	CN_1	
T4; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T4_2)	job_SP_699	CN_1	
T4; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T4_3)	job_SP_700	CN_1	
T4; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T4_4)	job_SP_701	CN_1	
T5; conformer I	BP86/def-TZVP	job_GEO_448	job_SP_453	CN_1	
T5; conformer I	BP86/def-TZVP	job_GEO_465	job_SP_466	CN_1	
T5; conformer I	BP86/def-TZVP	job_GEO_442	job_SP_461	CN_1	
T5; conformer I	BP86/def-TZVP	job_GEO_447	job_SP_456	CN_1	
T5; conformer II	BP86/def-TZVP	job_GEO_409	job_SP_423	CN_1	
T5; conformer II	BP86/def-TZVP	job_GEO_414	job_SP_427	CN_1	
T5; conformer II	BP86/def-TZVP	job_GEO_415	job_SP_430	CN_1	
T5; conformer II	BP86/def-TZVP	job_GEO_418	job_SP_432	CN_1	
T5; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T5_1)	job_SP_689	CN_1	
T5; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T5_2)	job_SP_690	CN_1	
T5; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T5_3)	job_SP_691	CN_1	
T5; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T5_4)	job_SP_692	CN_1	
T5; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T5_1)	job_SP_702	CN_1	
T5; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T5_2)	job_SP_703	CN_1	
T5; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T5_3)	job_SP_704	CN_1	
T5; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T5_4)	job_SP_705	CN_1	
T6; conformer I	BP86/def-TZVP	job_GEO_438	job_SP_457	CN_1	
T6; conformer I	BP86/def-TZVP	job_GEO_441	job_SP_462	CN_1	
T6; conformer I	BP86/def-TZVP	job_GEO_444	job_SP_463	CN_1	COSMO-BP-TZVPD-FINE_178
T6; conformer I	BP86/def-TZVP	job_GEO_445	job_SP_464	CN_1	
T6; conformer II	BP86/def-TZVP	job_GEO_411	job_SP_425	CN_1	
T6; conformer II	BP86/def-TZVP	job_GEO_412	job_SP_426	CN_1	
T6; conformer II	BP86/def2-TZVPP	job_GEO_560	job_SP_602	CN_1	COSMO-BP-TZVPD-FINE_93
T6; conformer II	BP86/def-TZVP	job_GEO_417	job_SP_431	CN_1	
T6; conformer II	BP86/def-TZVP	job_GEO_420	job_SP_435	CN_1	
T6; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T6_1)	job_SP_693	CN_1	COSMO-BP-TZVPD-FINE_180
T6; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T6_2)	job_SP_694	CN_1	
T6; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T6_3)	job_SP_695	CN_1	
T6; conformer III	BP86/def2-TZVPP	job_GEO_866	job_SP_892	CN_1	
T6; conformer III	BP86/def2-TZVPPD	job_GEO_867	job_SP_893	CN_1	
T6; conformer III	B3LYP/6-311+G(d,p)	JOB_1027		CN_GAU	
T6; conformer III	G4(MP2)	JOB_1027_1		CN_GAU	
T6; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T6_4)	job_SP_696	CN_1	
T6; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T6_1)	job_SP_706	CN_1	
T6; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T6_2)	job_SP_707	CN_1	
T6; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T6_3)	job_SP_708	CN_1	COSMO-BP-TZVPD-FINE_182
T6; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T6_4)	job_SP_709	CN_1	
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Anion					
	BP86/def-TZVP	job_GEO_539	job_SP_545	CN_3	
	B3LYP/def2-TZVPPD	job_GEO_561	job_SP_605	CN_1	COSMO-BP-TZVPD-FINE_95
	B3LYP/6-311+G(d,p)	JOB_1029		CN_GAU	
Neutral					
C-N-H	BP86/def-TZVP	job_GEO_540	job_SP_546	CN_3	
H-C-N	BP86/def-TZVP	job_GEO_541	job_SP_547	CN_3	
	B3LYP/def2-TZVPPD	job_GEO_562	job_SP_606	CN_1	COSMO-BP-TZVPD-FINE_97
	B3LYP/6-311+G(d,p)	JOB_1030		CN_GAU	
16					
Anion					
	BP86/def-TZVP	job_GEO_542	job_SP_548	CN_3	
	B3LYP/def2-TZVPPD	job_GEO_563	job_SP_607	CN_1	COSMO-BP-TZVPD-FINE_99
	B3LYP/6-311+G(d,p)	JOB_1031		CN_GAU	
Neutral					
T1; C(CN)2=CH(CN)	BP86/def-TZVP	job_GEO_552	job_SP_553	CN_3	
	B3LYP/def2-TZVPPD	job_GEO_564	job_SP_608	CN_1	COSMO-BP-TZVPD-FINE_101
	B3LYP/6-311+G(d,p)	JOB_1032		CN_GAU	
T4; C(CN-H)2=C(CN)	BP86/def-TZVP	job_GEO_544	job_SP_550	CN_3	
T6; C(CN)2=C(CN-H)	BP86/def-TZVP	job_GEO_477	job_SP_483	CN_1	
T5; C(CN-H)2=C(CN)	BP86/def-TZVP	job_GEO_478	job_SP_484	CN_1	

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Dianion

[B12(CN)12]2-

BP86/def-TZVP
BP86/def-TZVP
B3LYP/def2-TZVPPD
B3LYP/6-311+G(d,p)job_GEO_364
job_GEO_486
job_GEO_565
JOB_1033job_SP_369
job_SP_487
job_SP_594CN_3
CN_1
CN_1
CN_GAU

COSMO-BP-TZVPD-FINE_103

Anion

[B12(CN)12]-, protonated on CN

BP86/def-TZVP
B3LYP/def2-TZVPPD
B3LYP/6-311+G(d,p)job_GEO_365
job_GEO_566
JOB_1034job_SP_370
job_SP_597CN_3
CN_1
CN_GAU

COSMO-BP-TZVPD-FINE_105

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Neutral

B12(CN)12H2, H-s dide by side

B12(CN)12H2, 1 B between two H-s

B12(CN)12H2, 2 B-s between two H-s

BP86/def-TZVP
BP86/def-TZVP
BP86/def-TZVP
BP86/def-TZVP
B3LYP/def2-TZVPPD
B3LYP/6-311+G(d,p)job_GEO_373
job_GEO_376
job_GEO_488
job_GEO_372
job_GEO_567
JOB_1035job_SP_379
job_SP_380
job_SP_537
job_SP_381
job_SP_593CN_3
CN_3
CN_1
CN_3
CN_1
CN_GAU

COSMO-BP-TZVPD-FINE_107

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Anion

[CB11(CN)12]-

BP86/def-TZVP
B3LYP/def2-TZVPPD
B3LYP/6-311+G(d,p)job_GEO_391
job_GEO_568
JOB_1036job_SP_396
job_SP_592CN_3
CN_1
CN_GAU

COSMO-BP-TZVPD-FINE_109

Neutral

CB11(CN)12-H, H on CN that is on C

CB11(CN)12-H, H on CN that is on 1st row B

CB11(CN)12-H, H on CN that is on 2nd row B

CB11(CN)12-H, H on CN that is on opposite C

BP86/def-TZVP
BP86/def-TZVP
BP86/def-TZVP
BP86/def-TZVP
B3LYP/def2-TZVPPD
B3LYP/6-311+G(d,p)job_GEO_392
job_GEO_393
job_GEO_394
job_GEO_395
job_GEO_569
JOB_1037job_SP_397
job_SP_398
job_SP_399
job_SP_400
job_SP_596CN_3
CN_3
CN_3
CN_3
CN_1
CN_GAU

COSMO-BP-TZVPD-FINE_111

Compd name	CAS	FILENAME		NEUTRAL	
		ANION			
NH2-TCNP	98555-43-2		COSMO-BP-TZVPD-FINE_184	T4	COSMO-BP-TZVPD-FINE_186
				T5	COSMO-BP-TZVPD-FINE_188
Me-TCNP	24943-63-3		COSMO-BP-TZVPD-FINE_192	T3	COSMO-BP-TZVPD-FINE_190
				T4	COSMO-BP-TZVPD-FINE_194
3,4-(MeO)2-C6H3-TCNP	1261286-75-2	Conf 1	COSMO-BP-TZVPD-FINE_198	T5	COSMO-BP-TZVPD-FINE_196
				T4	COSMO-BP-TZVPD-FINE_289
		Conf 2	T5	COSMO-BP-TZVPD-FINE_202	
			T4	COSMO-BP-TZVPD-FINE_204	
			T5	COSMO-BP-TZVPD-FINE_304	
			T4	COSMO-BP-TZVPD-FINE_210	
4-MeO-C6H4-TCNP	1261286-76-3		COSMO-BP-TZVPD-FINE_208	T5	COSMO-BP-TZVPD-FINE_212
				T4	COSMO-BP-TZVPD-FINE_216
Ph-TCNP	96463-47-7		COSMO-BP-TZVPD-FINE_214	T5	COSMO-BP-TZVPD-FINE_219
				T4	COSMO-BP-TZVPD-FINE_225
3-CF3-C6H4-TCNP	2226486-85-5	Conf 1	COSMO-BP-TZVPD-FINE_223	T5	COSMO-BP-TZVPD-FINE_227
				T4	COSMO-BP-TZVPD-FINE_229
		Conf 2	T5	COSMO-BP-TZVPD-FINE_233	
			T3	COSMO-BP-TZVPD-FINE_237	
			T4	COSMO-BP-TZVPD-FINE_239	
			T4	COSMO-BP-TZVPD-FINE_245	
H-TCNP	32019-26-4		COSMO-BP-TZVPD-FINE_235	T5	COSMO-BP-TZVPD-FINE_247
				T4	COSMO-BP-TZVPD-FINE_251
Br-TCNP	100125-09-5		COSMO-BP-TZVPD-FINE_243	T5	COSMO-BP-TZVPD-FINE_253
				T4	COSMO-BP-TZVPD-FINE_258
3,5-(CF3)2-C6H3-TCNP	1261286-79-6		COSMO-BP-TZVPD-FINE_249	T5	COSMO-BP-TZVPD-FINE_260
				T4	COSMO-BP-TZVPD-FINE_276
Cl-TCNP	1261286-80-9		COSMO-BP-TZVPD-FINE_256	T5	COSMO-BP-TZVPD-FINE_278
				T4	COSMO-BP-TZVPD-FINE_264
CN-CH2-TCNP	2638-14-4		COSMO-BP-TZVPD-FINE_274	T5	COSMO-BP-TZVPD-FINE_266
				T4	COSMO-BP-TZVPD-FINE_264
CF3-TCNP	1261286-81-0		COSMO-BP-TZVPD-FINE_221	T4	COSMO-BP-TZVPD-FINE_264
				T5	COSMO-BP-TZVPD-FINE_266