

Supporting Information for

Oxidative cage opening in the C₇₀ fullerene facilitated by preceding trifluoromethylation

Sofia V. Gracheva, Nadezhda B. Tamm, Konstantin A. Lyssenko, Ilya N. Ioffe,
Natalia S. Lukonina,* and Alexey A. Goryunkov

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Reagents and solvents

C₇₀ (Fullerene-center, Russia, 99,8%), CF₃I (P&M Invest, Russia, 99%), pyridine (Acros Organics, 99+%), 18-crown-6 (Sigma-Aldrich, 99%) were used as received. K₂CO₃ was dried in vacuo at 120°C for 3 hours.

Toluene (Himed, 99%) was refluxed over Na for 2 h, and then distilled; fraction with b.p. 110.6 °C was collected. Hexane (Himed, 99%) was refluxed over P₂O₅ for 2 h, and then distilled; fraction with b.p. 69°C was collected.

o-Dichlorobenzene (Acros Organics, 99%) was refluxed over CaH₂ for 2 h, and then distilled under reduced pressure (12 mmHg); fraction with b.p. 64°C was collected.

Synthetic procedures

Trifluoromethylated fullerene C₅-C₇₀(CF₃)₈ was synthesized according to the two-step protocol involving trifluoromethylation of C₇₀ with CF₃I at the first stage followed by transalkylation the obtained product with C₇₀ at the second stage (see refs^{1,2}). Isomerically pure trifluoromethylfullerene was isolated by means of preparative HPLC using toluene as an eluent.

C₅-C₇₀(CF₃)₈: MALDI MS *m/z* (*I*, %): 1392 (M⁻, C₇₀(CF₃)₈⁻, 100%); HPLC (*t_R*, min, CB 4.6 mm i.d. × 250 mm, toluene 1 mL·min⁻¹): 4.6.

Synthesis of C₇₀(CF₃)₈(O)O₂ and C₆₉O(CF₃)₈O: K₂CO₃, pyridine (200 μL) and catalytic amount of 18-crown-6 were added to a solution of C₅-C₇₀(CF₃)₈ (6.5 mg, 4.7 μmol) in *o*-DCB (10 mL). The reaction mixture was refluxed under air atmosphere for 3 h. Then it was quenched by adding trifluoroacetic acid (300 μl), and filtered through a short plug of silica with toluene as an eluent. Semi-preparative HPLC separation of the reaction mixture using pure toluene as an eluent has yielded fractions with individual C₇₀(CF₃)₈(O)O₂ (**2a**, major) and C₆₉O(CF₃)₈O (**2b**, minor). Their yields were estimated by means of the HPLC trace integration (Figure S1). The isolated individual fractions were analyzed with the use of the LC-MS system (Figure S2). The mass spectra of compounds recorded with an APCI (atmospheric pressure chemical ionization) ion source reveal molecular ions and pseudomolecular ions with two additional OH-groups. Such mass spectral pattern is typical for C₅-C₇₀(CF₃) and its derivatives when an APCI ion source is used.

C₇₀(CF₃)₈(O)O₂: 30% yield, HPLC (*t_R*, min, CB 4.6 mm i.d. × 250 mm, toluene, 1 mL·min⁻¹): 7.6; APCI MS (negative mode) *m/z* (*I*, %): 1440 (44%, [C₇₀(CF₃)₈(O)O₂]⁻), 1474 (100%, [C₇₀(CF₃)₈(O)O₂(OH)₂]⁻); UV (*λ*_{max}, nm, cyclohexane): 308, 398, 420, 440.

C₆₉O(CF₃)₈O: 10% yield, HPLC (*t_R*, min, CB 4.6 mm i.d. × 250 mm, toluene, 1 mL·min⁻¹): 6.1; APCI MS (negative mode) *m/z* (*I*, %): 1412 (44%, [C₆₉O(CF₃)₈O]⁻), 1446 (100%, [C₆₉O(CF₃)₈O(OH)₂]⁻); UV (*λ*_{max}, nm, cyclohexane): 398, 434, 465.

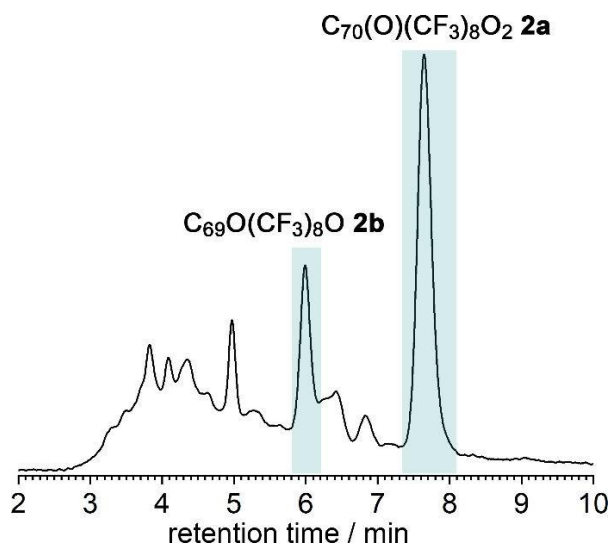


Figure S1. The HPLC trace of the reaction mixture (CB 4.6 mm i.d. \times 250 mm, toluene 1 mL \cdot min $^{-1}$). Isolated fractions of compounds **2a** and **2b** are highlighted.

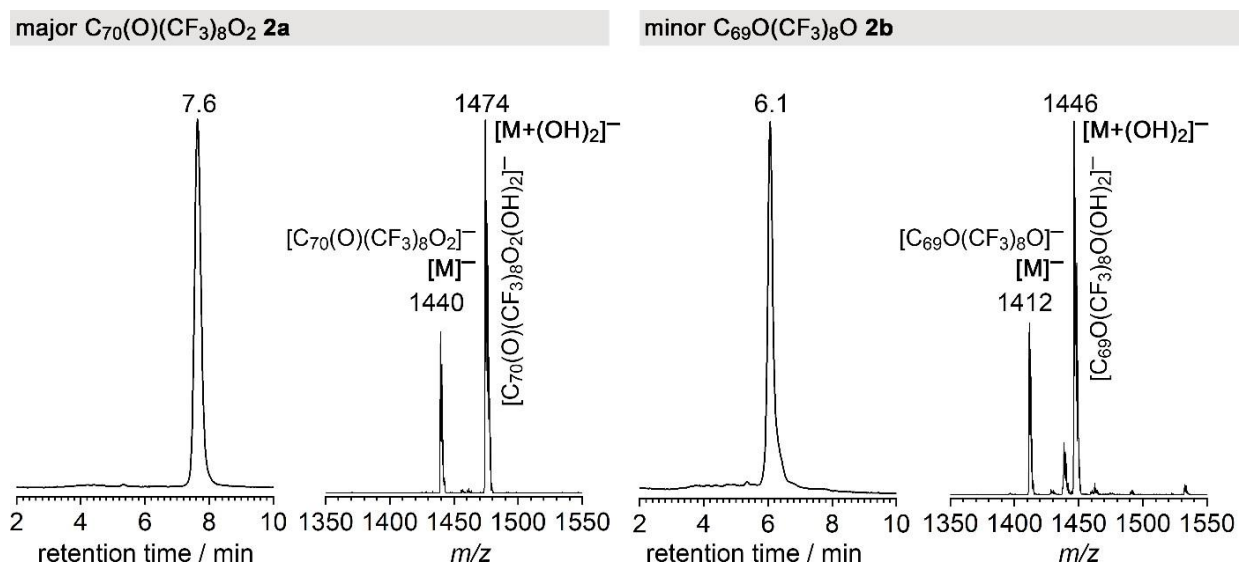


Figure S2. The HPLC traces (CB 4.6 mm i.d. \times 250 mm, toluene 1 mL \cdot min $^{-1}$) and the APCI mass spectra of compounds **2a** and **2b**.

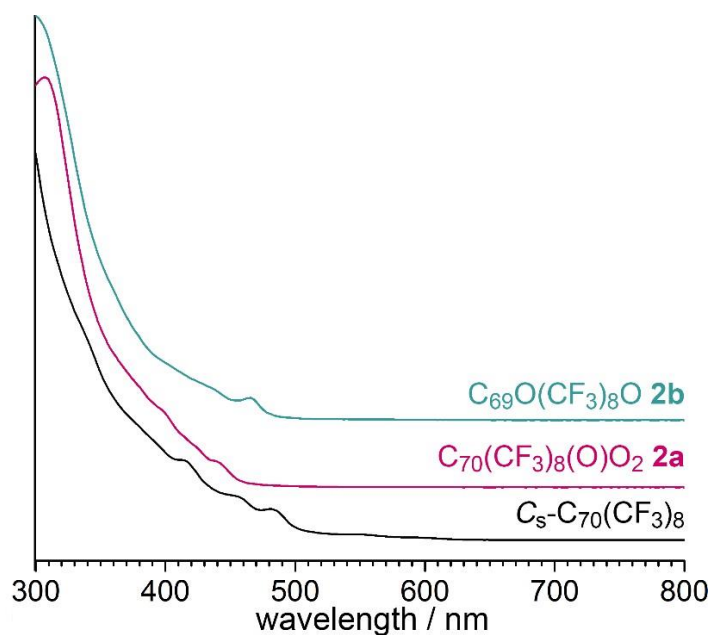


Figure S3. The UV-Vis spectra of C_5 - $C_{70}(CF_3)_8$ and its derivatives **2a** and **2b**.

Single crystal X-ray analysis

Single crystals of compounds **2a** and **2b** were obtained via slow evaporation of toluene from HPLC-isolated fractions. They were investigated with a Bruker D8 QUEST single-crystal X-ray diffractometer equipped with PHOTON II detector, charge-integrating pixel array detector (CPAD), laterally graded multilayer (Goebel) mirror and microfocus Mo-target X-ray tube ($\lambda = 0.73071 \text{ \AA}$). Data reduction and integration were performed with the Bruker software package SAINT (Version 8.40B).³ The data were corrected for Lorentz and polarization effects. The absorption correction was performed using multiscan routine as implemented in SADABS (Version 2016/2).⁴ Crystal structure solution and refinement were performed using SHELX-2018 package.⁵ Atomic positions were located using dual method and refined using a combination of Fourier synthesis and least-square refinement in isotropic and anisotropic approximations. The contribution of strongly disordered toluene molecule for the structural amplitudes in **2a** were excluded by the SQUEEZE method in the PLATON program,⁶ which substantially improved the model. The analysis of Fourier synthesis has revealed that in **2b** the oxygen atoms are disordered over two positions with occupancies 0.26 and 0.74. Upon refinement, the EADP and EXYZ routines (for atom in the fullerene fragment) were used. An additional epoxy oxygen was found at one of the poles in **2b** with the occupancy 0.21 (apparently, this additional oxidation occurred in the course of crystal growth). Crystallographic parameters and final residuals for the single-crystal XRD experiment are given in Table S1.

Table S1. Crystallographic data for compounds **2a** and **2b**.

	Compound 2a	Compound 2b
Formula	$C_{85}H_8F_{24}O_3$	$C_{84}H_8F_{24}O_{2.21}$

FW	1532.91	1508.22
<i>T</i> , K	100	120
Crystal system	Monoclinic	Monoclinic
Space group	<i>P2₁/c</i>	<i>P2₁/c</i>
<i>Z</i> (<i>Z'</i>)	4(1)	4(1)
<i>a</i> , Å	11.2201(4)	20.2976(7)
<i>b</i> , Å	22.3582(8)	18.2848(7)
<i>c</i> , Å	21.7383(8)	14.2099(5)
β , °	101.3429(12)	99.129(2)
<i>V</i> , Å ³	5346.8(3)	5207.0(3)
<i>d</i> _{calc} , g·cm ⁻³	1.904	1.924
μ , cm ⁻¹	1.73	1.75
F(000)	3032	2983
2 θ _{max} , °	60	52
Measured refl.	57312	43812
Independent refl.	15671	9679
Observed refl.	9166	5048
Parameters	946	1025
<i>R</i> ₁ for observed refl.	0.0693	0.0823
<i>wR</i> ₂ for all refl.	0.1847	0.2057
GOF	0.970	1.033
Peak and hole, e·Å ⁻³ (<i>d</i> _{min} / <i>d</i> _{max})	0.535/−0.350	0.603/−0.562

Experimental methods

High-Performance Liquid Chromatography–Mass spectrometry. Analyses of samples were performed using LC-MS system equipped with Agilent 1100 (diode array detector operated at 190–950 nm), a Cosmosil Buckyprep column (4.6 mm i.d. × 250 mm) at 23°C, mass-selective 6410 Triple Quadrupole LC/MS detector (Agilent Technologies, Inc.), and the APCI (Atmospheric Pressure Chemical Ionization) ion source. Isolation of the compounds was performed using Waters Breeze series system (UV/vis λ 2 detector operated at 190–700 nm) equipped with a Cosmosil Buckyprep semi-preparative column (10 mm i.d. × 250 mm) at 25°C. Toluene was used as an eluent.

Fluorescence spectroscopy. Absorption and emission spectra were recorded using ULS2048x64TEC SensLine fiber-optic spectrometer equipped with AvaLight-DHc light source (200–2500 nm range,

deuterium and halogen lamps). Spectrometer working range is 190–1100 nm. Optical resolution is 0.04 nm. Samples were measured at the 355 nm excitation using light-emitting diode source AvaLight-LED355 (FWHM=10 nm). Fluorescence quantum yields were determined by the relative method with respect to the quinine sulfate reference (QS ($\geq 98\%$, BioReagent, Sigma-Aldrich) in 0.5M H₂SO₄ (Φ_F 0.546)).⁷ For each sample, 5–10 measurements with various concentrations of analyte were performed. The absorbance remained within 0.1 arb. units at the excitation wavelength (355 nm) for all samples. The resulting Φ_F value was obtained from a linear approximation of the integral fluorescence and absorption data from all measurements according to the equation:⁸

$$\Phi_{sm} = \Phi_{ref} \cdot \frac{F_{sm}}{F_{ref}} \cdot \frac{A_{ref}}{A_{sm}} \cdot \frac{n_{ref}^2}{n_{sm}^2}$$

where *sm* denotes sample and *ref* – the reference; *F* is the relative integral photon flux for spectrally corrected and blank-corrected spectra; *A* is integral absorbance in the range of 355±0.5 nm; *n* is refractive index of the solvent. In the equation, we used *A* instead of the absorption factor *f* since it offers a good approximation for very dilute solutions.⁹

Quantum chemical calculations

Optimization of the stable structures and transition states, as well as verification of the latter by means of the IRC tracking were carried out at the DFT level of the theory using of the PRIRODA v.6 software that features an efficient RI approximation.¹⁰ PBE exchange-correlation functional¹¹ and a built-in valence- and core-split augmented basis set L22a with contraction scheme (13s,9p,6d,3f)/[7s,6p,4d,2f] for the first-row atoms were used. The vibrational calculations and the respective geometry optimizations employed a reduced TZ2p basis set with contraction scheme (10s,3p,3d,1f)/[6s,3p,2d] for the first-row atoms. To our experience, the two basis sets give only marginal differences in vibrational calculations, and the PBE xc functional does not require frequency scaling. In the transition state structures below, the imaginary frequency and the respective mode are given. Because of the condensed-phase conditions, the free energy values presented below exclude the translational contributions.

Due to the compatibility issues of the visualization software, the molecular orbitals were recalculated at the PBE/Def2-TZVPP level using the ORCA software,¹² v. 5.0.4.

DFT is known to systematically overestimates the triplet-singlet gap in O₂ by 50-60 kJ mol⁻¹, and our tests reveal that the thermochemistry of simple reactions with oxygen is better reproduced with the singlet O₂ taken as the computational reference and the triplet O₂ placed 94 kJ mol⁻¹ below, in accordance with the well-known experimental triplet-singlet gap in O₂. Therefore, the data for the Path A below are calculated with respect to the (**1** + singlet O₂) effective transition state denoted below as **T-S**(¹O₂) whose energy is set at +94 kJ mol⁻¹, and the energy of the starting (**1** + triplet O₂) system is taken to be zero.

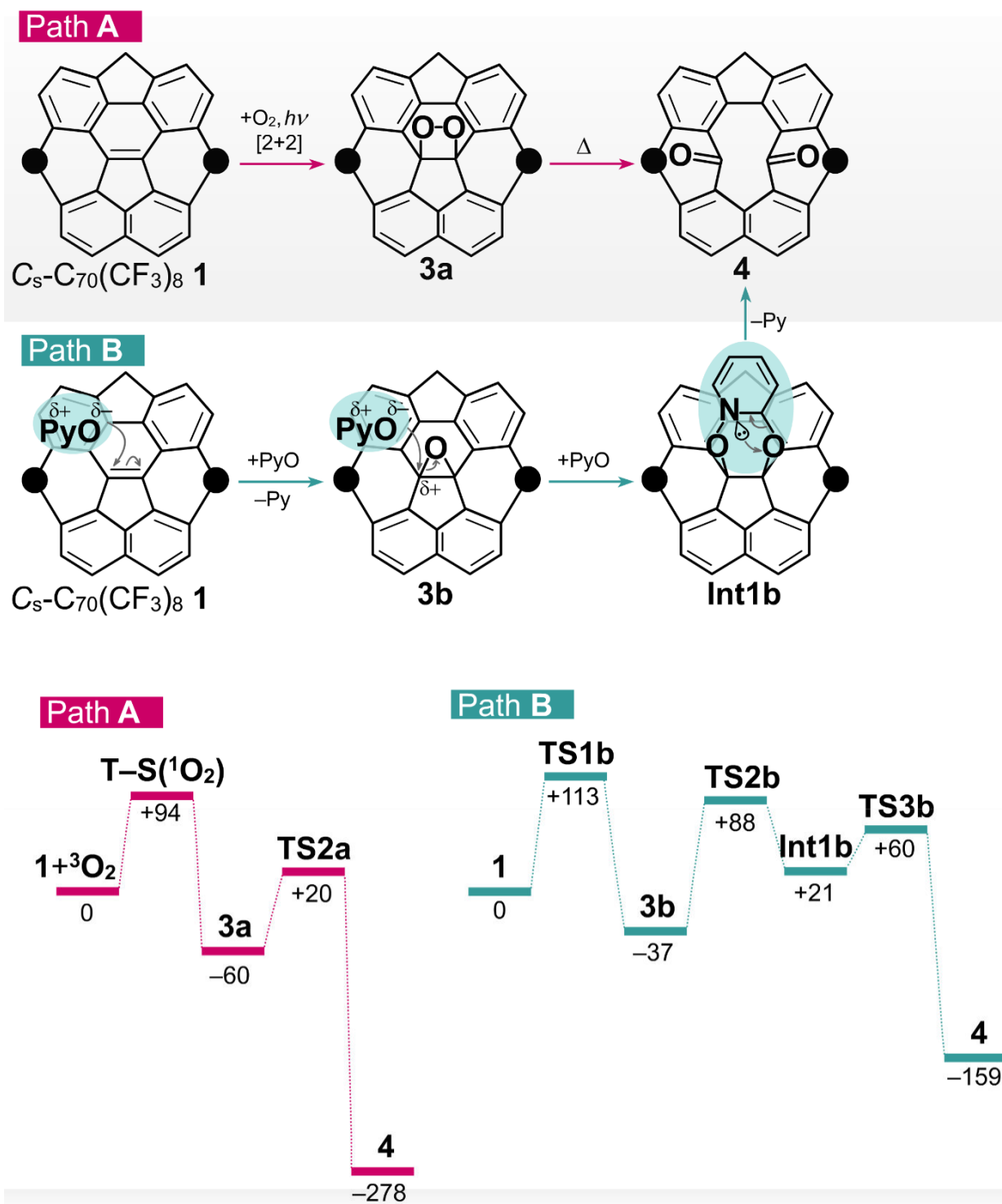
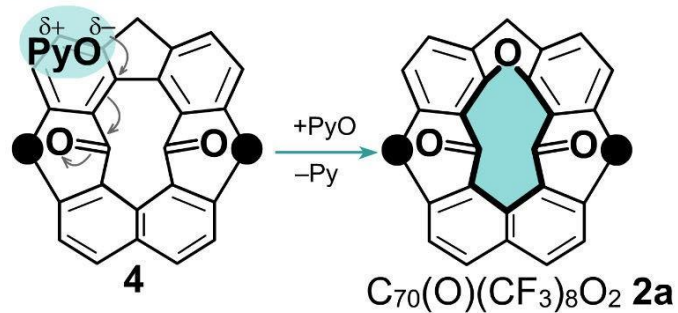
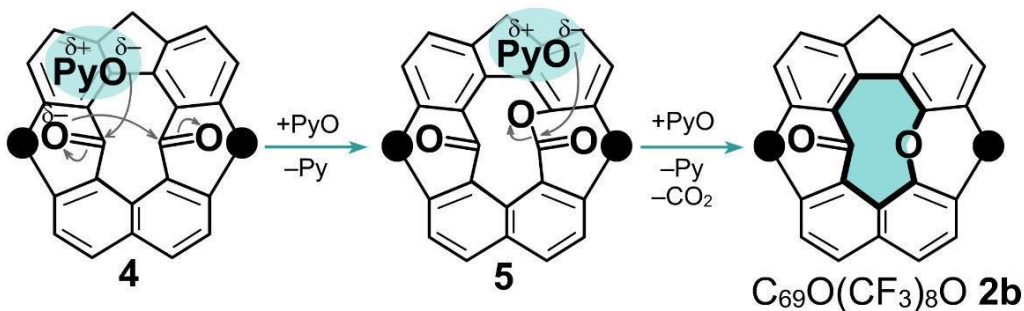


Figure S4. The mechanism of compounds **2a** and **2b** formation from $C_S-C_{70}(CF_3)_8$ (depicted in the Figure 2).

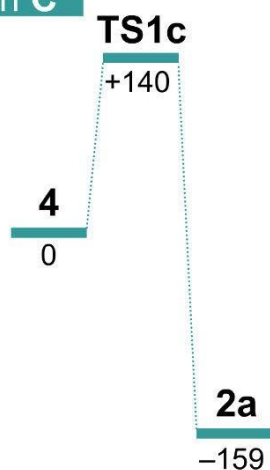
Path C



Path D



Path C



Path D

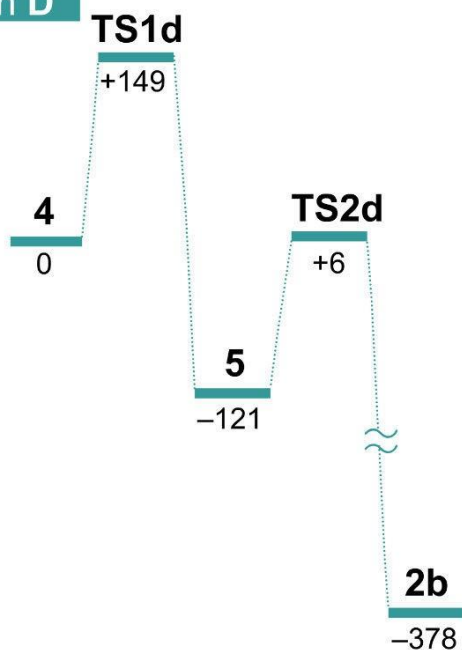


Figure S4 (continuation). The mechanism of compounds **2a** and **2b** formation from C_5 - $C_{70}(CF_3)_8$ (depicted in the Figure 2). The potential energy profile between intermediate **5** and product **2b** is actually more complex, with extra saddle points separated from each other by very shallow (some 10 kJ mol^{-1}) local minima. Here we provide the data for the highest of the saddle points.

Table S2. Calculated energy levels of intermediates and transitions states (TS) of proposed pathways formation of products **2a** and **2b**.

Process	Electronic energy + ZPVE ΔE (0 K), kJ mol ⁻¹	Free energy ΔG (453 K), kJ mol ⁻¹	Process	Electronic energy + ZPVE ΔE (0 K), kJ mol ⁻¹	Free energy ΔG (453 K), kJ mol ⁻¹
Path A			Path C		
1+³O₂	0	0	4	0	0
T-S(¹O₂)	94	94	TS1c	132	140
3a	-71	-60	2a	-161	-159
TS2a	12	20	Path D		
4	-280	-278	4	0	0
Path B			TS1d	137	149
1	0	0	5	-123	-121
TS1b	105	113	TS2d	-5	6
3b	-39	-37	2b	-372	-378
TS2b	80	88			
Int1b	1	21			
TS3b	47	60			
4	-153	-159			

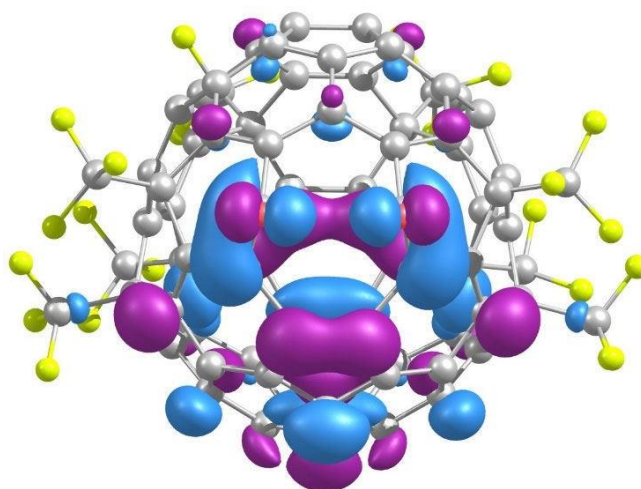
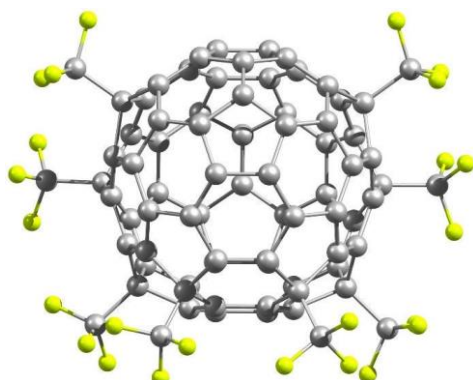


Figure S5. The LUMO distribution in diketone C₇₀(CF₃)₈O₂ (**4**).

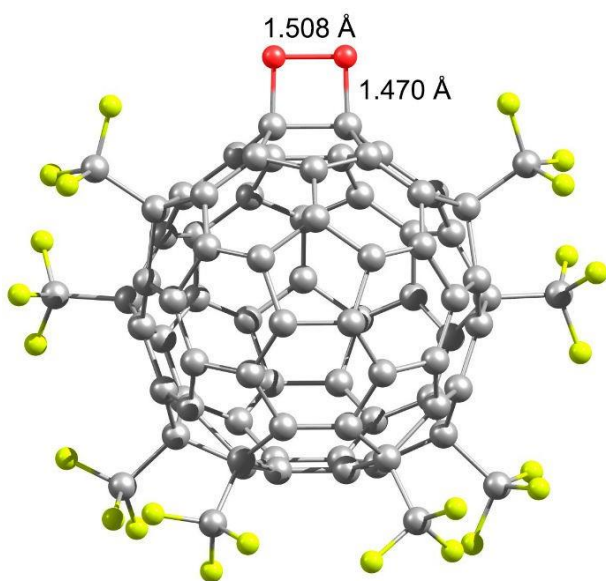
Atomic coordinates of the optimized structures

Compound 1, $C_{5-C70}(CF_3)_8$



N	X	Y	Z	N	X	Y	Z
9	-4.1112727	-2.898636	-3.08027288	6	-1.63008141	-2.5719675	-1.55734964
9	-3.92782692	-0.95604293	-4.08536171	6	-2.33137764	-2.78901838	-0.3482791
9	-2.48520831	-2.5403536	-4.5027493	6	-1.67443769	-3.34586928	0.75817956
9	1.65326964	-3.91022797	-4.32276004	6	-2.00120418	-2.88411276	2.08980788
9	0.18834771	-2.60708305	-5.26966987	6	-2.98284869	-1.90186922	2.28270644
9	-0.47297217	-4.2907635	-4.02069816	6	-2.73159762	-0.83898958	3.22447976
9	1.74000074	-5.95980005	-0.11423271	6	-3.2402766	0.38563395	2.65796449
9	2.36143785	-5.26157347	-2.07858136	6	-2.50132851	1.56608289	2.82009432
9	3.75054501	-5.12310457	-0.38668049	6	-2.32826654	2.47974248	1.71205074
9	0.60171948	-4.81947369	4.16532889	6	-2.89198985	2.17566856	0.4653787
9	-0.55831864	-5.83408464	2.59930994	6	-2.20249677	2.50675418	-0.72435462
9	1.62343474	-5.67017645	2.44205561	6	-2.69464669	1.56597557	-1.86416396
9	-1.76105384	4.34849116	4.34885813	6	-1.47565817	0.99329909	-2.5867733
9	0.31714805	4.9263257	3.96322841	6	-1.31086808	-0.42219002	-2.8158205
9	-0.12149192	3.37545405	5.43942214	6	-0.06056765	-0.92561034	-3.17120323
9	0.21291141	6.00349274	1.48616921	6	0.47507523	-2.35551871	-2.86789302
9	1.67467969	6.02139623	-0.13252628	6	-0.28324488	-2.91873175	-1.66423225
9	2.33074435	5.59675085	1.90387591	6	0.39631703	-3.48474101	-0.52161151
9	-1.75382695	4.55985925	-3.1144112	6	-0.30202757	-3.68758238	0.67007608
9	0.25136867	4.39083626	-3.98148384	6	0.31275705	-3.6405985	2.09856764
9	-0.07086538	5.56237158	-2.15473914	6	-0.79454267	-2.88896226	2.85038401
9	-4.81754608	1.44543336	-3.04043644	6	-0.53824089	-1.85490574	3.72353769
9	-4.21319167	3.40916852	-2.31160276	6	-1.51583217	-0.81721757	3.92875406
9	-3.21367852	2.51782922	-4.05460568	6	-0.79331598	0.41810029	4.09834904
6	-3.33707549	-1.77039628	-0.15815063	6	-1.29901845	1.59474158	3.58964511
6	-3.6617187	-1.33302297	1.12921771	6	-0.40848217	2.7621528	3.14310915
6	-3.82030562	0.07665401	1.36046221	6	-1.06682421	3.11965677	1.78418651
6	-3.64739109	0.95810799	0.28905317	6	-0.38245819	3.46763355	0.61961825
6	-3.39484283	0.48507544	-1.04103732	6	-0.96787361	3.15066049	-0.66295785
6	-3.24354059	-0.8579213	-1.26117211	6	-0.14956484	3.17146368	-1.95088289
6	-2.34522545	-1.44267076	-2.35012713	6	-0.37452777	1.83997123	-2.72026055
				6	0.88360153	1.32024269	-3.09833789
				6	1.03911436	-0.05270077	-3.32491089
				6	2.2649057	-0.71519663	-2.9406346
				6	1.9224334	-2.03052139	-2.49463823
				6	2.57285156	-2.56879225	-1.41347757
				6	1.9221348	-3.55751134	-0.44424806
				6	2.4024532	-2.97208012	0.91536833
				6	1.62566607	-2.86315738	2.05817814
				6	1.86636315	-1.76814133	2.98616977
				6	0.79539109	-1.25591031	3.78694841
				6	0.63983786	0.13098886	4.01558503

Compound 3a, C_s-C₇₀(CF₃)₈(O₂)

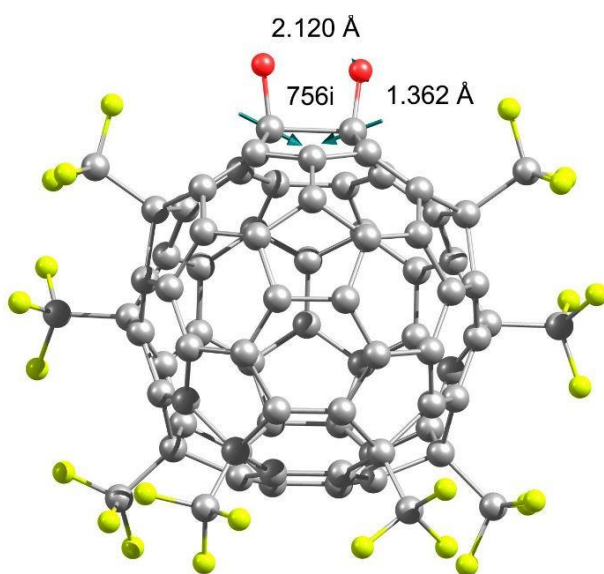


N	X	Y	Z
6	-1.19815254	0.62289438	3.73405481
6	-0.02754054	1.37941443	3.60435253
6	1.24321096	0.67200087	3.9860777
6	1.24577569	-0.91400776	3.93667412
6	-0.02254634	-1.59791863	3.51028077
6	-1.19544863	-0.85466636	3.68747062
6	-2.41611776	-1.26110693	3.07354782
6	-3.19458397	-0.08826696	2.74455611
6	-2.42026878	1.06454476	3.14776734
6	-2.41367564	2.21779599	2.34815328
6	-1.22371759	2.97340926	2.17568788
6	-0.04269804	2.56863608	2.80085567
6	1.25384077	3.20775104	2.32327865
6	2.41928891	2.21597641	2.37039358
6	2.41623766	1.07911113	3.14211554
6	3.14669007	-0.07950417	2.712693
6	2.42059533	-1.26594534	3.0693648
6	2.42837456	-2.3528237	2.22799542
6	1.26244513	-3.33744141	2.10959604
6	-0.0338546	-2.7316897	2.63006281
6	-1.21193786	-3.09388163	1.97890457
6	-2.40560327	-2.3600908	2.20180406
6	-3.19821621	-2.33304351	0.99483854
6	-3.96999384	-1.20192001	0.68926473
6	-3.95890136	-0.05379095	1.57988014
6	-3.97395831	1.14766118	0.76377726
6	-3.20361574	2.25867381	1.13972085
6	-2.48615731	3.03271924	0.17249742

N	X	Y	Z
6	-1.31205578	3.75633911	0.83510617
6	-0.019426	3.55225139	0.04598409
6	1.16001067	3.46071021	0.78916545
6	2.3436105	2.97604922	0.18065031
6	3.13739712	2.23891725	1.13765258
6	3.91400888	1.15047042	0.72729613
6	3.9198827	-0.04026683	1.53541954
6	3.91789569	-1.17715878	0.6531262
6	3.14466935	-2.2916737	0.99379957
6	2.35136985	-2.9649176	-0.00931127
6	1.16907297	-3.48965509	0.56631774
6	-0.01069356	-3.54616255	-0.17769754
6	-1.30337341	-3.80636395	0.60080498
6	-2.4778124	-3.04550315	-0.01797267
6	-2.4817112	-2.5741315	-1.30735585
6	-3.20305453	-1.37761901	-1.61919921
6	-3.97412131	-0.71131489	-0.66079875
6	-3.97627613	0.74222853	-0.61434705
6	-3.21011748	1.47031856	-1.53040588
6	-2.4893647	2.64380939	-1.14326421
6	-1.32867424	2.89320028	-2.10784228
6	-0.02913862	3.14821259	-1.34122266
6	1.14263872	2.66091602	-1.92086205
6	2.33400911	2.57938067	-1.16369089
6	3.12781821	1.45035217	-1.59328073
6	3.9101276	0.74888028	-0.66863268
6	3.91244914	-0.68702882	-0.71441712
6	3.13519982	-1.33189689	-1.68377437
6	2.34365881	-2.48711608	-1.32648495
6	1.1518231	-2.5222513	-2.08635211
6	-0.01517412	-3.04852457	-1.53438005
6	-1.31265874	-2.74723577	-2.27962978
6	-1.23027209	-1.31980578	-2.88960059
6	-2.4161057	-0.62180695	-2.56528808
6	-2.41993893	0.77821189	-2.52162756
6	-1.23611468	1.49967289	-2.79649357
6	-0.06566904	0.82272195	-3.1324404
6	1.22498503	1.63514649	-3.08561428
6	2.40192286	0.77561539	-2.62445837
6	2.40424828	-0.59660297	-2.66826557
6	1.23613397	-1.43085243	-3.19495457
6	-0.05988199	-0.62073116	-3.18363678
6	1.6371649	4.43744407	3.21287981
9	2.11540431	4.0009425	4.4111081
9	2.60947332	5.17799889	2.62299386

N	X	Y	Z	N	X	Y	Z
9	0.59235654	5.24832732	3.48269636	6	-1.65762597	-3.8443031	-3.33137662
6	1.62644376	-4.64059923	2.88288967	9	-1.88203313	-5.03647731	-2.72614193
9	1.92907903	-4.34259656	4.17493917	9	-2.77918493	-3.51073958	-4.02206273
9	0.6122052	-5.53424865	2.90148649	9	-0.65996669	-4.02843887	-4.22538955
9	2.70875593	-5.24691132	2.33160644	6	1.56116865	2.28582487	-4.46080948
6	-1.66176512	5.27342064	0.9886328	9	0.57160073	3.09401335	-4.9027028
9	-2.62691901	5.45235209	1.92670146	9	2.69611538	3.02769288	-4.37691892
9	-0.59348638	6.02530066	1.33302237	9	1.75688839	1.33112483	-5.40452659
9	-2.12963996	5.76984975	-0.18575271	6	1.60366957	-2.01081358	-4.62431836
6	-1.65655921	-5.3434035	0.7261571	9	2.04954662	-3.28976963	-4.5314651
9	-0.57339812	-6.13400348	0.54675182	9	0.55261072	-1.98620164	-5.47514494
9	-2.18641815	-5.61989514	1.94609166	9	2.59981551	-1.29007194	-5.20175257
9	-2.57967477	-5.71282967	-0.19714451	8	1.48239641	-0.91974271	5.38708469
6	-1.71171318	4.0580049	-3.1158662	8	1.48022721	0.58797331	5.43415172
9	-2.7500155	4.79433108	-2.64357951				
9	-0.68221793	4.91015186	-3.32706265				
9	-2.10507261	3.55701725	-4.31486528				

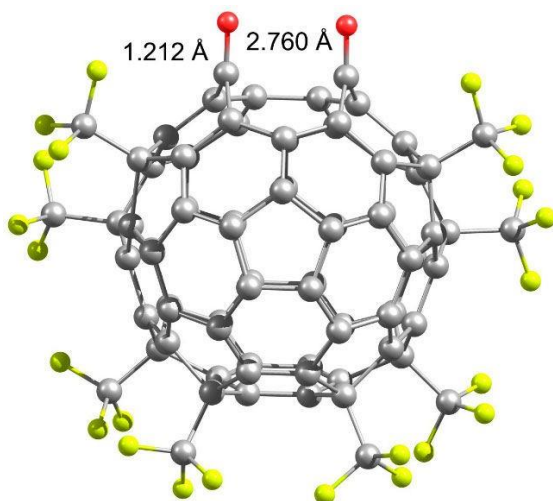
Transition state TS2a, C₇₀(CF₃)₈(O...O)



N	X	Y	Z	N	X	Y	Z
6	-1.19864878	0.63306184	3.73296475	6	-1.23064103	2.98718623	2.16820956
6	-0.03237716	1.39617236	3.58637037	6	-0.05173258	2.58259944	2.78878014
6	1.2239309	0.7424742	4.07431982	6	1.25188956	3.20778445	2.3281385
6	1.31650345	-1.01895928	4.0135117	6	2.40473822	2.19532465	2.3874332
6	-0.01100871	-1.59760736	3.53771825	6	2.41560578	1.06266554	3.17804504
6	-1.18222388	-0.84342183	3.69522044	6	3.13915376	-0.09450411	2.72511241
6	-2.40305754	-1.25230459	3.07461237	6	2.4239276	-1.29179035	3.05396002
6	-3.18858572	-0.08415457	2.74350325	6	2.43649773	-2.37256818	2.20908611
6	-2.41958947	1.07055494	3.14406643	6	1.26604167	-3.34717981	2.10302926
6	-2.41826615	2.22459351	2.34371216	6	-0.02238725	-2.72462463	2.63570571
				6	-1.19969789	-3.07880682	1.9779643
				6	-2.39574857	-2.3495912	2.20348264
				6	-3.19169103	-2.32607687	0.99844957
				6	-3.96761113	-1.19829676	0.6913635
				6	-3.95668347	-0.05087715	1.58069013
				6	-3.97520895	1.15021585	0.76348316
				6	-3.20729866	2.26436237	1.13769796
				6	-2.49023263	3.03949788	0.16883384
				6	-1.31744636	3.76718328	0.82962052
				6	-0.02043873	3.55737972	0.04720443
				6	1.15802793	3.45941108	0.79414011
				6	2.33717371	2.9644549	0.19049127
				6	3.11819504	2.2169284	1.14952685
				6	3.90305114	1.13860639	0.7359934
				6	3.90953588	-0.05056104	1.5417951
				6	3.91462006	-1.18318853	0.65149487
				6	3.14760249	-2.30682831	0.98046932
				6	2.35306554	-2.97833047	-0.02233198

6	1.16971212	-3.49742365	0.55800259	9	0.60270951	5.25852656	3.47260327
6	-0.01062006	-3.54772315	-0.18372174	6	1.62511563	-4.65622946	2.87134222
6	-1.29863748	-3.79857646	0.60167897	9	1.95803675	-4.36557791	4.15437018
6	-2.47334029	-3.03874006	-0.01532871	9	0.59688009	-5.53396882	2.90796973
6	-2.48095771	-2.570631	-1.3059585	9	2.68617247	-5.27823131	2.29495062
6	-3.20318697	-1.37481376	-1.61800141	6	-1.66732677	5.28432778	0.9773688
6	-3.9741483	-0.70914369	-0.65954373	9	-2.64275414	5.46413383	1.90449379
6	-3.97723728	0.74427163	-0.61405374	9	-0.60265817	6.03527151	1.3327457
6	-3.21047278	1.47251956	-1.53049217	9	-2.12202558	5.77867741	-0.20306703
6	-2.49105142	2.64761734	-1.14529568	6	-1.65818628	-5.33386005	0.73417268
6	-1.32859325	2.8964201	-2.10797945	9	-0.57905427	-6.12972325	0.55658256
6	-0.02909978	3.15068581	-1.33906045	9	-2.1896178	-5.60287125	1.95449758
6	1.143078	2.66070662	-1.91625376	9	-2.58286694	-5.70139416	-0.18868211
6	2.33198653	2.57462806	-1.15606947	6	-1.71065332	4.06079716	-3.11753112
6	3.12580022	1.44712259	-1.58712772	9	-2.75802582	4.78905191	-2.65284756
6	3.90575028	0.74434376	-0.66306346	9	-0.68490067	4.91968056	-3.31800757
6	3.91020606	-0.69073442	-0.71368853	9	-2.09064971	3.55943492	-4.32058271
6	3.13442157	-1.33486568	-1.68656993	6	-1.66274589	-3.84127309	-3.33261944
6	2.34359894	-2.49358315	-1.33600609	9	-1.88922678	-5.0325029	-2.72658759
6	1.15032827	-2.52321581	-2.09339591	9	-2.78385451	-3.50529702	-4.02255275
6	-0.01651874	-3.04820245	-1.53941136	9	-0.665737	-4.02741503	-4.22694818
6	-1.31453948	-2.7446653	-2.28112429	6	1.56548694	2.29038839	-4.45580265
6	-1.23161577	-1.31701217	-2.89035885	9	0.58112764	3.1071846	-4.89300868
6	-2.41682538	-0.61903872	-2.56525726	9	2.70537744	3.02408558	-4.36938245
6	-2.42014433	0.78092685	-2.52168018	9	1.75384453	1.33830409	-5.40342005
6	-1.23605369	1.5025369	-2.79576997	6	1.59995845	-2.00609344	-4.62964605
6	-0.06549179	0.82534087	-3.13198211	9	2.04888168	-3.28401552	-4.53913384
6	1.22605577	1.63658719	-3.08265532	9	0.54640022	-1.98307254	-5.47731907
6	2.40142293	0.77495851	-2.62184517	9	2.59269062	-1.28210891	-5.20838551
6	2.40379635	-0.59703848	-2.66971641	8	1.71080132	-1.22262538	5.30041161
6	1.23460903	-1.42891332	-3.19858819	8	1.25511634	0.84335474	5.43283022
6	-0.06075497	-0.6178352	-3.18462215				
6	1.64343838	4.43874697	3.21252897				
9	2.11658092	4.00829598	4.41249682				
9	2.6212033	5.1687035	2.61723129				

Compound 4, $C_5-C_{70}(CF_3)_8(O)_2$

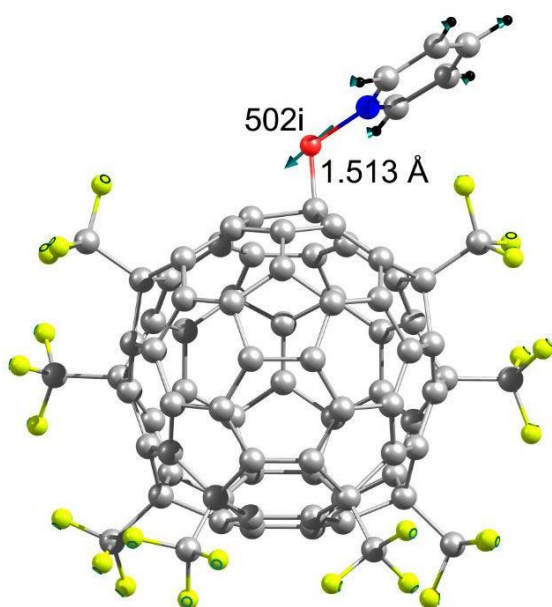


N	X	Y	Z
6	-0.81486747	3.14750128	2.22775765
6	0.55021413	3.02406153	2.55514694
6	1.04131668	2.42743174	3.85465532
6	-1.09956605	0.75246673	4.48317076
6	-1.99424645	1.03222299	3.29689475
6	-1.97557555	2.23809333	2.56685489
6	-2.90009943	2.35099027	1.47598866
6	-2.41580748	3.29215216	0.50330207
6	-1.12728999	3.73885235	0.95890891
6	-0.12190952	4.01074105	0.0152601
6	1.23309586	3.71636133	0.30094504
6	1.56033995	3.22004489	1.55603965
6	2.90948459	2.52850555	1.72658814
6	2.78386931	1.29717658	2.64933261
6	1.78888937	1.14357716	3.60000722
6	1.2791578	-0.18304195	3.90563937
6	-0.13899514	-0.36686736	4.16868009
6	-0.78637851	-1.49666563	3.69705107
6	-2.25511275	-1.50752127	3.22332568
6	-2.69844651	-0.11189742	2.79372527
6	-3.52375252	-0.00582992	1.68491531
6	-3.6556965	1.24803256	1.0448631
6	-3.91613369	1.05105838	-0.36301867
6	-3.44894126	1.98014131	-1.30133097
6	-2.68843717	3.13218358	-0.85423113
6	-1.64425427	3.38969686	-1.8273706
6	-0.38036193	3.80924026	-1.39238885
6	0.81922982	3.3038487	-1.98970105
6	1.99340646	3.43974285	-1.02018817
6	2.7559673	2.1224876	-0.88251118
6	3.27671077	1.82500713	0.38106569

6	3.70323405	0.50671815	0.66798172
6	3.4170093	0.18511403	2.04534626
6	3.07527034	-1.10730358	2.42629119
6	1.9843009	-1.29154972	3.34683033
6	1.30347639	-2.49353838	2.94270476
6	-0.08005456	-2.54953538	3.06487993
6	-0.89799069	-3.08704088	2.00484699
6	-2.13228602	-2.39889652	1.95222589
6	-2.75338535	-2.17524406	0.72079612
6	-3.8807225	-1.13949859	0.69285221
6	-3.8756158	-0.35823615	-0.62127502
6	-3.28324975	-0.81516505	-1.77236135
6	-2.73399867	0.12090788	-2.70554652
6	-2.84797742	1.5025328	-2.51575308
6	-1.73085479	2.37476093	-2.84071792
6	-0.54495497	1.83142576	-3.34612009
6	0.73727606	2.32167189	-2.94409483
6	1.8027286	1.24161051	-3.14405498
6	2.66372699	1.0863091	-1.88704192
6	3.09184113	-0.20619079	-1.5816426
6	3.61699165	-0.49814104	-0.30245013
6	3.28631841	-1.85146041	0.08372472
6	3.03690381	-2.15972017	1.4269226
6	1.93781319	-3.01912488	1.74673989
6	1.14935159	-3.52628427	0.70605328
6	-0.29011123	-3.55340378	0.83402703
6	-0.90251105	-3.32700443	-0.41919403
6	-2.11876788	-2.64902002	-0.48837724
6	-2.5365707	-2.14824974	-1.86896055
6	-1.27034135	-1.71317874	-2.65975784
6	-1.50536954	-0.43640143	-3.22052604
6	-0.43008977	0.40427036	-3.53511833
6	0.89655769	-0.01702588	-3.28823612
6	1.14068636	-1.27698692	-2.74618837
6	2.54552902	-1.5217914	-2.20268795
6	2.50912028	-2.42648789	-0.97014901
6	1.45450109	-3.25111414	-0.6634455
6	0.19506866	-3.3723025	-1.52348458
6	0.03378865	-2.14875544	-2.42561085
6	4.00252074	3.47980875	2.31638185
9	3.7927995	3.64673071	3.65112149
9	5.24244503	2.95138109	2.15548637
9	3.99106905	4.70944977	1.76159686
6	-3.16460528	-2.10419169	4.33605167
9	-3.03346803	-1.38427724	5.48116964
9	-4.47210342	-2.08858715	3.99208644
9	-2.81955152	-3.38828222	4.61069195

6	2.92009062	4.60520385	-1.49414297	9	-3.71520648	-2.74299334	-3.87587087
9	2.28998631	5.80097399	-1.36671496	9	-2.78741568	-4.38366194	-2.75915627
9	4.08021607	4.66432401	-0.80530151	6	3.4960367	-2.13454208	-3.27443023
9	3.2452236	4.44479063	-2.80280883	9	3.62124096	-1.3414505	-4.36187462
6	-5.312612	-1.76105219	0.95720328	9	4.73779252	-2.32983708	-2.75903417
9	-5.2400064	-2.98342644	1.53259726	9	3.02746662	-3.33477501	-3.6978738
9	-6.04826538	-0.95495237	1.76558267	6	0.22641334	-4.74330489	-2.31987886
9	-6.0088668	-1.9011835	-0.19898255	9	-0.513172	-5.69040716	-1.68806894
6	2.64082814	1.55089505	-4.45706889	9	-0.23647161	-4.61390501	-3.58377514
9	2.47205145	2.83771185	-4.85544357	9	1.49221	-5.22825806	-2.4062603
9	3.96754861	1.36025073	-4.27192348	8	-1.2182009	1.31224618	5.5519678
9	2.23689088	0.76942033	-5.49098057	8	0.89870044	2.97028201	4.9295259
6	-3.40988171	-3.19008314	-2.63019037				
9	-4.57415532	-3.41076181	-1.97048799				

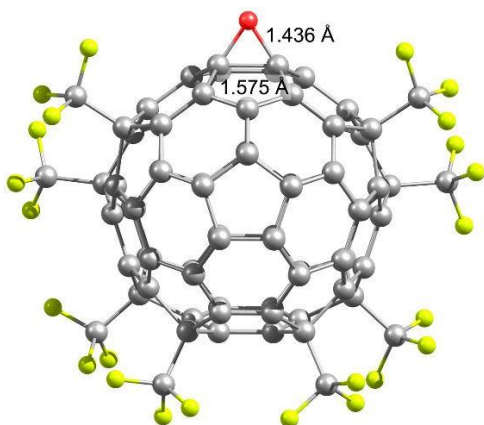
Transition state TS1b, C₇₀(CF₃)₈...O...Py



N	X	Y	Z				
9	-4.18802477	-2.60883093	-3.8526735	9	0.05355402	5.48847576	3.02465319
9	-3.94494505	-0.7130527	-4.93105315	9	-0.49355339	4.01894545	4.54599599
9	-2.49963564	-2.32297978	-5.21739372	9	0.0559116	6.45330028	0.50078197
9	1.60088855	-3.7456442	-4.78560659	9	1.57991947	6.37667114	-1.05677806
9	0.20458502	-2.4660928	-5.85916393	9	2.1487839	6.03822758	1.02091081
9	-0.54279675	-4.07733548	-4.56462025	9	-1.73261255	4.81831105	-4.12034731
9	1.48246494	-5.58076604	-0.44490322	9	0.30534237	4.58261667	-4.88889058
9	2.14009968	-5.01797207	-2.4415341	9	-0.07908797	5.84647358	-3.13786451
9	3.51003178	-4.79765513	-0.74333034	9	-4.83926322	1.74515535	-4.03877052
9	0.03102129	-4.33863307	3.65151553	9	-4.24198685	3.73468722	-3.37885922
9	-0.83317744	-5.39160476	1.93443573	9	-3.17729006	2.74823649	-5.02884077
9	1.3373594	-5.1198597	2.09921601	6	-3.5306505	-1.3455194	-0.94910322
9	-2.05452321	4.97799179	3.33515086	6	-3.90159173	-0.84566632	0.30337773
				6	-4.05035782	0.57522395	0.46554829
				6	-3.82773969	1.40455989	-0.64164925
				6	-3.52107854	0.8661126	-1.93147279
				6	-3.38170895	-0.48949339	-2.08819214
				6	-2.44251246	-1.13346007	-3.10833374
				6	-1.77677545	-2.23277709	-2.23375214
				6	-2.53068312	-2.38256199	-1.04638122
				6	-1.92598284	-2.88775392	0.11364388
				6	-2.29983235	-2.36449859	1.40719199
				6	-3.27429387	-1.36624768	1.50753148
				6	-3.04653206	-0.26409962	2.40637849
				6	-3.52806817	0.93770042	1.76925169
				6	-2.7735346	2.11273504	1.90826006
				6	-2.54982762	2.97749089	0.76841541
				6	-3.06106648	2.61937329	-0.48624105
				6	-2.31613816	2.88816276	-1.65789806
				6	-2.76897408	1.89841095	-2.77261398
				6	-1.52683588	1.27848876	-3.41268042

6	-1.37331436	-0.14838692	-3.57223651	6	3.06832309	1.69154522	-2.7588363
6	-0.11560176	-0.68175968	-3.8499721	6	3.21805347	0.25473466	-2.92238618
6	0.38681643	-2.10348488	-3.46034335	6	3.84688206	-0.26515644	-1.7387136
6	-0.43107004	-2.5996628	-2.26640859	6	3.41226072	-1.50016161	-1.23261871
6	0.19152362	-3.11460577	-1.06962921	6	3.21790427	-1.67195063	0.18832603
6	-0.55785022	-3.24778133	0.10000602	6	3.47442488	-0.60634254	1.05954191
6	-0.00611391	-3.15193762	1.55294415	6	2.58867337	-0.38188332	2.16301973
6	-1.12774135	-2.35223564	2.22867468	6	2.45732272	1.05724449	2.34085148
6	-0.90379753	-1.30323935	3.08880029	6	3.24042476	1.68787553	1.32978403
6	-1.85868844	-0.23020447	3.15726844	6	2.75640513	2.84504454	0.70109961
6	-1.12491444	1.00597472	3.2928281	6	2.93905651	3.0283774	-0.71298409
6	-1.61645144	2.17288869	2.73327928	6	3.61107433	2.05550832	-1.47735495
6	-0.68993184	3.30247511	2.26880354	6	4.08482883	0.84673681	-0.83526465
6	-1.28447728	3.60694753	0.86746673	6	3.90239845	0.67069102	0.53933979
6	-0.5446393	3.89126172	-0.28058949	6	-3.27260829	-1.7051871	-4.29460036
6	-1.07675371	3.52049778	-1.57162741	6	0.40201081	-3.11410844	-4.68219356
6	-0.20044393	3.46865995	-2.81991444	6	2.21321775	-4.66903734	-1.13139527
6	-0.40974501	2.10477635	-3.53587702	6	0.14101918	-4.52093871	2.29374083
6	0.85802262	1.55371821	-3.83394857	6	-0.79415491	4.46932115	3.29584656
6	1.00265904	0.1694858	-3.99376576	6	1.17379027	5.79994457	0.10407436
6	2.20091865	-0.48984796	-3.52764532	6	-0.43577304	4.69201407	-3.7541058
6	1.82242286	-1.78072619	-3.040642	6	-3.7610662	2.54525141	-3.82490117
6	2.41846397	-2.2776057	-1.90884019	6	1.83197766	-4.5675262	6.7549734
6	1.70869763	-3.20716872	-0.92130339	6	2.805728	-3.90124867	6.00720657
6	2.13644004	-2.56447803	0.42893256	6	2.49301036	-2.6716592	5.43203435
6	1.30556632	-2.37408476	1.53601911	7	1.26342221	-2.16833813	5.59131416
6	1.53295876	-1.27581974	2.43673513	6	0.29950622	-2.77575291	6.29117898
6	0.48495991	-0.76508441	3.38608714	6	0.56560698	-3.99509307	6.90652755
6	0.28486955	0.72647478	3.36020335	1	2.05845175	-5.52748472	7.21797086
6	1.21936137	1.61066721	2.75632921	1	3.80354902	-4.31597939	5.87329464
6	0.75717994	2.83827812	2.11716746	1	3.19523866	-2.06576968	4.86070835
6	1.50331097	3.40745572	1.10043986	1	-0.65863779	-2.25929782	6.34037209
6	0.93122638	4.24886438	-0.07689449	1	-0.21390078	-4.48301372	7.4894827
6	1.78833757	3.71603399	-1.22597598	8	0.88228517	-0.74646094	4.84562323
6	1.28242113	3.37230064	-2.45305354				
6	1.90579143	2.32460842	-3.20758558				

Compound 3b, C₅-C₇₀(CF₃)₈O



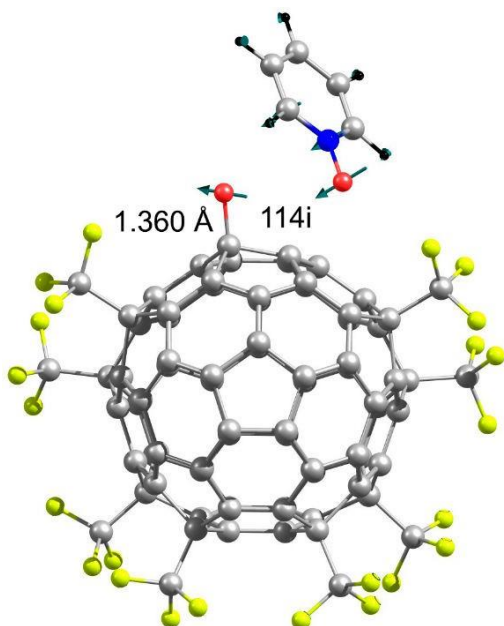
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9	-2.50148641	-2.53350552	-4.55394132
9	1.63581149	-3.90581028	-4.38031573
9	0.1687989	-2.60272778	-5.3235448
9	-0.4894371	-4.28650978	-4.07345178
9	1.72073749	-5.95380468	-0.16985246
9	2.34623554	-5.25824579	-2.13351039
9	3.73369637	-5.12279545	-0.44039046
9	0.60941415	-4.80548411	4.11373525
9	-0.55149265	-5.82691775	2.55321595
9	1.62862822	-5.64954231	2.38596806
9	-1.75712918	4.36415496	4.2955722
9	0.32342329	4.93016753	3.9044742
9	-0.12025437	3.38321306	5.38258433
9	0.19687319	6.01215761	1.43069474
9	1.65043139	6.03505287	-0.19475684
9	2.31762461	5.61083507	1.8377669
9	-1.7724096	4.56254066	-3.17311534
9	0.23065703	4.39222666	-4.04431542
9	-0.08817759	5.56953997	-2.22105913
9	-4.833868	1.44767844	-3.09018026
9	-4.22728192	3.41355813	-2.37012995
9	-3.23079185	2.51475237	-4.11073812
6	-3.34771481	-1.76316258	-0.20814856
6	-3.66884929	-1.32434005	1.08100466
6	-3.82746984	0.0841788	1.31092714
6	-3.65838579	0.96534661	0.23702474
6	-3.40899243	0.491772	-1.09087334
6	-3.25736147	-0.85320673	-1.310376
6	-2.35945215	-1.43748228	-2.40075823
6	-1.64357084	-2.56749092	-1.60975135
6	-2.34235981	-2.7827544	-0.39935403

N	X	Y	Z
6	-1.6824978	-3.33504173	0.70740284
6	-2.00502764	-2.86883501	2.03634584
6	-2.98390742	-1.88994315	2.23208724
6	-2.72681577	-0.82740745	3.17209596
6	-3.24118593	0.39422311	2.60497946
6	-2.50477897	1.57225404	2.76163337
6	-2.3369129	2.48729973	1.65642737
6	-2.90375733	2.18454896	0.41104504
6	-2.2168957	2.515439	-0.77985659
6	-2.7090965	1.5713262	-1.91700334
6	-1.48961989	0.99860159	-2.63905382
6	-1.32465158	-0.41766221	-2.86722857
6	-0.07509463	-0.92107182	-3.22385379
6	0.4610921	-2.35138961	-2.92221049
6	-0.29640169	-2.91410578	-1.71760137
6	0.38462691	-3.47737768	-0.57486346
6	-0.31083461	-3.67827458	0.61991751
6	0.30385506	-3.62948778	2.04967309
6	-0.79862651	-2.87292307	2.79972953
6	-0.54954875	-1.86484965	3.6978713
6	-1.50759597	-0.80475203	3.87729275
6	-0.80848994	0.43930542	4.07598496
6	-1.3023464	1.60017746	3.5332764
6	-0.41761533	2.77016024	3.08895386
6	-1.0762707	3.12832708	1.72891882
6	-0.39503603	3.47670289	0.56146223
6	-0.98205971	3.15986191	-0.7202
6	-0.16442726	3.17917553	-2.00888014
6	-0.38934698	1.84533928	-2.77460995
6	0.86939151	1.32553421	-3.15340617
6	1.0250571	-0.04783785	-3.37915136
6	2.25059596	-0.71034425	-2.99656902
6	1.90959602	-2.02686085	-2.55217318
6	2.56145262	-2.5657298	-1.47223343
6	1.90946606	-3.55180893	-0.50137839
6	2.38766789	-2.96062233	0.85424103
6	1.60791978	-2.8407876	2.00140105
6	1.87188561	-1.78165242	2.94138442
6	0.83208626	-1.34676533	3.88719536
6	0.65864292	0.19767406	4.1404363
6	1.54535876	1.12053173	3.41614802
6	1.02386517	2.33600708	2.84510787
6	1.71651789	2.9703714	1.82041592
6	1.08164093	3.85435147	0.71198777
6	1.89344395	3.38879916	-0.4979234
6	1.33500198	3.08930873	-1.71535746

N	X	Y	Z
6	1.93471003	2.08245748	-2.53771613
6	3.1249432	1.44593686	-2.17183053
6	3.28544408	0.01999532	-2.40440622
6	3.97219724	-0.54382222	-1.27424534
6	3.57505932	-1.80535822	-0.80502293
6	3.45055984	-2.04529703	0.61327913
6	3.73318573	-1.01863755	1.52531518
6	2.90090665	-0.86244532	2.67716829
6	2.73894116	0.57667781	2.91284645
6	3.47606136	1.26237191	1.8978629
6	2.94523926	2.43558636	1.3447434
6	3.07084913	2.69273306	-0.07036686
6	3.71285205	1.75907963	-0.89791067
6	4.23195422	0.52761872	-0.33032701

N	X	Y	Z
6	4.11500528	0.28935805	1.04007596
6	-3.23865574	-1.96410338	-3.57411766
6	0.43357481	-3.30392545	-4.19146395
6	2.43166586	-4.99518827	-0.80381628
6	0.50662999	-5.00498033	2.76930819
6	-0.49204386	3.88663457	4.17382453
6	1.30664244	5.40128317	0.95468285
6	-0.45893233	4.44093805	-2.87464727
6	-3.75698852	2.25202468	-2.89288311
8	1.1636482	-0.71064041	5.13073577

Transition state TS2b, $C_{70}(CF_3)_8(O)...O...Py$

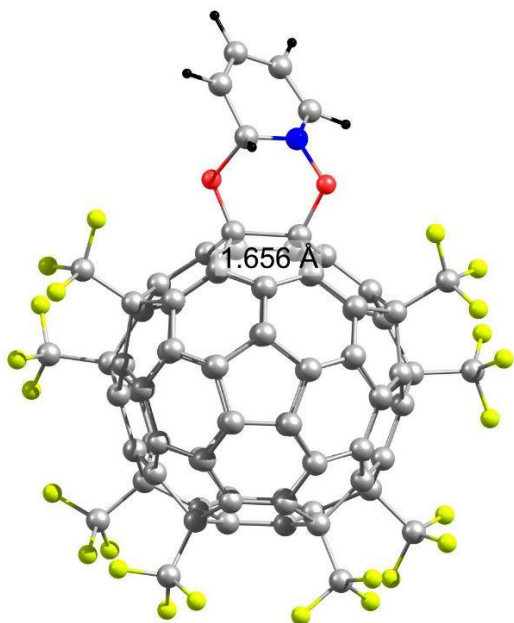


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9	-0.61360182	3.38367589	4.84190934
9	-0.01823518	6.18438582	1.0420383
9	1.51523296	6.24104622	-0.50733429
9	2.06705734	5.69843004	1.53108634
9	-1.81372668	5.03833525	-3.71088008
9	0.22597396	4.85937778	-4.48983794
9	-0.15534504	5.94487311	-2.62218036
9	-4.97637189	2.03629165	-3.91205812
9	-4.32828349	3.94022032	-3.07314024
9	-3.29639862	3.08960256	-4.81706659
6	-3.70982109	-1.37874704	-1.1737689
6	-4.07102436	-1.00148184	0.12759191
6	-4.19915931	0.39819108	0.43279184
6	-3.95912609	1.33053033	-0.58355293
6	-3.66431082	0.92218962	-1.92110958
6	-3.54652582	-0.41498222	-2.2152483
6	-2.61774663	-0.96431171	-3.29901488
6	-1.97312381	-2.16173125	-2.54656344
6	-2.73091238	-2.42098077	-1.38059044
6	-2.13856289	-3.05564091	-0.28167401
6	-2.49948058	-2.65705053	1.06207492
6	-3.45093913	-1.64805402	1.2654833
6	-3.20953106	-0.64585971	2.27600991
6	-3.66812841	0.61980601	1.76575737
6	-2.89988206	1.76131839	2.02570475
6	-2.65611444	2.72625226	0.97756879
6	-3.17497753	2.5123808	-0.30618791

N	X	Y	Z
9	-4.3751173	-2.33130855	-4.20332884
9	-4.12240936	-0.32434308	-5.05405973
9	-2.68793269	-1.89812627	-5.53120402
9	1.37370854	-3.48761807	-5.21076382
9	0.0514452	-2.04881188	-6.17427299
9	-0.78546197	-3.75287815	-5.0673258
9	1.32336335	-5.7107514	-0.96458212
9	1.77529534	-5.04309231	-2.99068178
9	3.30731735	-4.90051598	-1.42667755
9	-0.53149943	-5.01556057	3.00146949
9	-0.92684085	-5.83083656	1.01353331
9	1.135959	-5.46381762	1.67521462

N	X	Y	Z	N	X	Y	Z
6	-2.42654937	2.88607784	-1.44579875	6	1.78347321	2.41514276	-3.04542035
6	-2.8953683	2.02212995	-2.65428016	6	2.93442442	1.71979516	-2.66145197
6	-1.66296642	1.45110161	-3.35597353	6	3.06054144	0.30326647	-2.96698738
6	-1.53179079	0.04510787	-3.65917601	6	3.67477025	-0.34509688	-1.84362309
6	-0.28418298	-0.47910827	-3.99113466	6	3.22019788	-1.61965767	-1.467313101
6	0.19396694	-1.94187811	-3.75021508	6	3.02162922	-1.93453798	-0.07412649
6	-0.63401599	-2.5461979	-2.61560288	6	3.29284203	-0.96617254	0.90733891
6	-0.02329323	-3.19523969	-1.47866989	6	2.39793411	-0.8389245	2.0075831
6	-0.77724605	-3.43667899	-0.33105102	6	2.26701153	0.59331883	2.32072342
6	-0.22965638	-3.51047514	1.12485436	6	3.08341183	1.30264744	1.39639785
6	-1.33504195	-2.75712601	1.87325349	6	2.62596998	2.53070457	0.89291862
6	-1.0773467	-1.7736508	2.81942998	6	2.8237659	2.8542323	-0.49892786
6	-2.01835858	-0.69337461	3.01876897	6	3.47405641	1.94491303	-1.3487977
6	-1.29304739	0.50253839	3.33526909	6	3.92665284	0.66624153	-0.8296709
6	-1.73457638	1.70958045	2.85369209	6	3.73431313	0.35601924	0.5151057
6	-0.79972714	2.87602885	2.5101213	6	-3.45595842	-1.38922079	-4.54099691
6	-1.38173977	3.32136295	1.14094004	6	0.19739291	-2.82298979	-5.0681706
6	-0.63958742	3.71254456	0.02505418	6	1.97815748	-4.76566007	-1.67784443
6	-1.17713026	3.48572132	-1.29690069	6	-0.12904213	-4.97777872	1.70836403
6	-0.30297796	3.54917991	-2.54661807	6	-0.89394174	3.94403689	3.63951231
6	-0.53294082	2.26734362	-3.39534768	6	1.09544787	5.56178221	0.59145274
6	0.72565458	1.72804505	-3.74798698	6	-0.52068395	4.8635506	-3.35381112
6	0.84867286	0.36455401	-4.04674684	6	-3.87906464	2.7884242	-3.63389035
6	2.03250654	-0.35920092	-3.64777652	8	0.52847941	0.08972676	4.91979482
6	1.63337396	-1.68776666	-3.29859056	6	3.94535059	-1.93911615	6.99615045
6	2.21829698	-2.30949458	-2.22400933	6	4.12538963	-2.7570919	5.87462528
6	1.49305734	-3.3243296	-1.33913163	6	3.04408898	-3.07244063	5.07219773
6	1.92682922	-2.83461576	0.07045746	7	1.78984032	-2.59906873	5.37027786
6	1.10095691	-2.76865562	1.1882309	6	1.59583443	-1.79260857	6.46069227
6	1.32720762	-1.73925326	2.18444729	6	2.66467831	-1.46201305	7.27950576
6	0.25637894	-1.28154004	3.0304181	1	4.78825397	-1.68396479	7.63655747
6	0.17431606	0.1737756	3.60905997	1	5.10332103	-3.16104748	5.61792623
6	1.07042889	1.13128695	2.79834842	1	3.08284543	-3.70974716	4.19279864
6	0.63610953	2.40400322	2.30890589	1	0.5745397	-1.45409519	6.58981372
6	1.39783329	3.07747033	1.34891683	1	2.47762747	-0.81992312	8.13836266
6	0.83861419	4.03667988	0.25984557	8	0.78242898	-2.9040191	4.60037458
6	1.68915431	3.61120961	-0.93916447				
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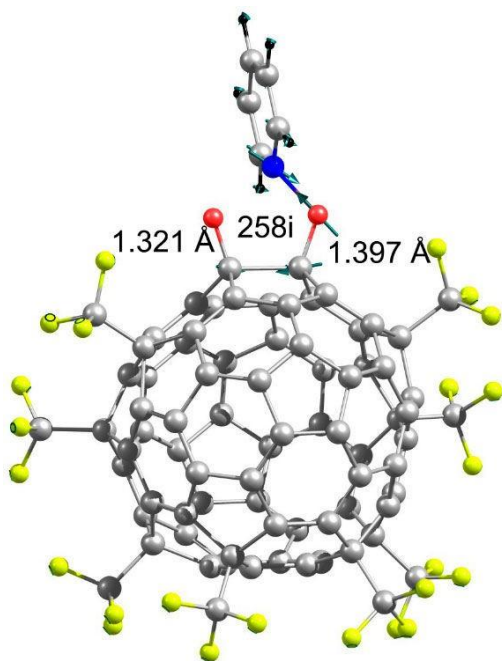


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6	-1.95839011	-2.22603487	-2.58095832
6	-2.69027846	-2.50900749	-1.40469107
6	-2.07465433	-3.17402957	-0.33595396
6	-2.39782535	-2.79714474	1.02064643
6	-3.34154394	-1.79842074	1.27451171
6	-3.05677986	-0.8237722	2.2924876
6	-3.51871324	0.45396871	1.82843997
6	-2.7361309	1.58086852	2.09974479
6	-2.51769997	2.57542858	1.07399547
6	-3.07109576	2.39824789	-0.20106867
6	-2.34830111	2.7961665	-1.34882674
6	-2.8524668	1.96632018	-2.56718512
6	-1.64088155	1.40348014	-3.31078254
6	-1.52715424	0.00420072	-3.65090728
6	-0.29165996	-0.51999867	-4.02434956
6	0.18071378	-1.99123775	-3.83223117
6	-0.62418333	-2.61796319	-2.69233971
6	0.00981632	-3.2986047	-1.58693538
6	-0.71658161	-3.56419342	-0.42598084
6	-0.13289871	-3.66485157	1.01500592
6	-1.2063162	-2.90901806	1.7973597
6	-0.92459795	-1.96545742	2.7550839
6	-1.84026353	-0.89786022	3.00148954
6	-1.10741058	0.27845239	3.34967584
6	-1.55473606	1.50245491	2.89964531
6	-0.62730646	2.6731386	2.56471646
6	-1.23831336	3.15915744	1.22111727
6	-0.52054265	3.57402252	0.09789307
6	-1.09114324	3.38395265	-1.21540716
6	-0.24594398	3.47161358	-2.48383155
6	-0.5059107	2.21205427	-3.35680621
6	0.73986132	1.67278727	-3.75244186
6	0.84590147	0.31649631	-4.08652417
6	2.03387461	-0.42549096	-3.73590039
6	1.632505	-1.75902431	-3.40880446
6	2.23864331	-2.41140385	-2.36470191
6	1.52671854	-3.44353708	-1.48744696
6	1.99875286	-2.98764229	-0.07575357
6	1.19918907	-2.93008689	1.0709565
6	1.46825469	-1.94953163	2.08921382
6	0.47138497	-1.62176148	3.19238663
6	0.36237591	-0.02369173	3.61325363
6	1.22788249	0.89818957	2.75235824

N	X	Y	Z
9	-4.41611879	-2.32479764	-4.17118838
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9	-2.74820946	-1.91244972	-5.5290254
9	1.32345764	-3.47505306	-5.38561147
9	-0.05938112	-2.03288789	-6.25163577
9	-0.82406956	-3.78052638	-5.15946395
9	1.2508464	-5.85275925	-1.32372909
9	1.89297879	-5.04378083	-3.23919191
9	3.29206635	-5.07995149	-1.55006259
9	-0.05547754	-5.07872842	2.95767786
9	-1.059032	-5.88624766	1.18234021
9	1.13052509	-5.73633325	1.25678169
9	-1.92336297	4.28291582	3.7923413
9	0.2135341	4.71859687	3.55815576
9	-0.42936166	3.13038633	4.91142272
9	0.1524587	6.00357971	1.18957044
9	1.62230782	6.10139097	-0.41829053
9	2.25315038	5.4918823	1.5784867
9	-1.7734575	5.00343582	-3.5678371
9	0.24079134	4.82086342	-4.41085446
9	-0.0736648	5.86679456	-2.50832929
9	-4.95597571	2.02309364	-3.78353165
9	-4.28619097	3.89965266	-2.89972457
9	-3.29060011	3.09932638	-4.68851842
6	-3.65920802	-1.46644178	-1.15021381
6	-3.98744093	-1.11861358	0.16563915
6	-4.09580912	0.27266565	0.50710906
6	-3.87094451	1.22935956	-0.48944806

N	X	Y	Z	N	X	Y	Z
6	0.79136389	2.18660612	2.30869807	6	0.14421153	-2.83498365	-5.17470083
6	1.53758657	2.88221808	1.3537297	6	1.99356058	-4.87805263	-1.89463929
6	0.96480294	3.8786528	0.30686462	6	-0.02082914	-5.11544244	1.59926772
6	1.78464702	3.4787616	-0.92265341	6	-0.68662855	3.72075349	3.71771329
6	1.24224579	3.29840979	-2.17044856	6	1.24376793	5.3903843	0.67469169
6	1.81902243	2.33423803	-3.05833678	6	-0.47245594	4.80669408	-3.25375963
6	2.97358551	1.62044477	-2.72002444	6	-3.85134853	2.76377018	-3.50397468
6	3.08256493	0.21155956	-3.06435093	8	0.80946841	0.29667534	4.93670701
6	3.71936881	-0.47041032	-1.97231435	6	2.88326092	-0.60896903	7.28474698
6	3.26491869	-1.7501677	-1.61782736	6	3.56432153	-1.4955262	6.38249945
6	3.09573843	-2.10112969	-0.2270332	6	2.82553898	-2.13686318	5.43129608
6	3.38832264	-1.15856169	0.76974094	7	1.46639759	-1.93905449	5.39173051
6	2.52891623	-1.0630886	1.90258038	6	0.81527033	-0.80400924	5.94625753
6	2.40844168	0.36629772	2.24204744	6	1.56528273	-0.31060052	7.13354463
6	3.20668375	1.09580958	1.31825398	1	3.43416062	-0.18948344	8.12772658
6	2.74755831	2.33831998	0.85712883	1	4.62269891	-1.71629326	6.48962543
6	2.92177137	2.70123124	-0.52899819	1	3.20753711	-2.88161483	4.73662808
6	3.54350869	1.8076533	-1.41473348	1	-0.23677383	-1.05898506	6.14768019
6	3.99879257	0.5120241	-0.93907419	1	1.0386398	0.35381006	7.81502767
6	3.82942484	0.16843911	0.40084451	8	0.72191242	-2.52550971	4.36030401
6	-3.48430411	-1.39818734	-4.5178242				

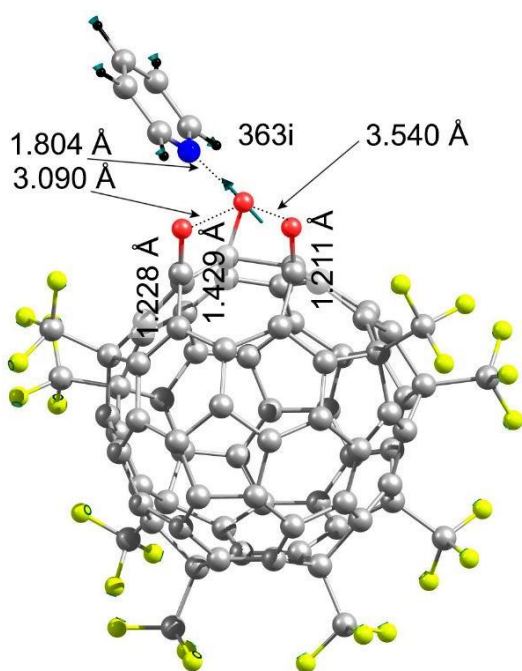
Transition state TS3b, $C_{70}(CF_3)_8(O)_2 \dots Py$



N	X	Y	Z	N	X	Y	Z
9	-4.44614835	-2.39706795	-4.10604694	9	-0.12087255	-2.14790058	-6.24388298
9	-4.18827414	-0.41013459	-5.00122366	9	-0.85860239	-3.86785258	-5.09139212
9	-2.79608699	-2.01703773	-5.49416807	9	1.26545824	-5.81987161	-1.23482483
9	1.28316247	-3.555131	-5.35610441	9	1.89156493	-5.05860078	-3.17424171
				9	3.30165649	-5.04504685	-1.49446862
				9	0.04597932	-4.91155802	3.05886867
				9	-1.03426764	-5.77714634	1.35635637
				9	1.15641495	-5.64351836	1.33748155
				9	-1.91184664	4.4247159	3.66021045
				9	0.20344043	4.91133133	3.35057138
				9	-0.35427593	3.34217342	4.76355957
				9	0.1403255	6.1145524	0.93160621
				9	1.62118249	6.15689635	-0.66833567
				9	2.23773287	5.61636895	1.35202862
				9	-1.82786669	4.96343223	-3.74213253
				9	0.17534541	4.76140735	-4.6059692
				9	-0.11644475	5.85837013	-2.72893935
				9	-4.99878264	1.96019741	-3.84565096
				9	-4.33101155	3.86351865	-3.02012683
				9	-3.34729754	3.01904383	-4.79471567
				6	-3.65946715	-1.44509915	-1.11964717
				6	-3.97349673	-1.06027486	0.18934462
				6	-4.08406158	0.33970935	0.49089522

6	-3.87685043	1.2680059	-0.53639905	6	0.40019601	0.21271365	3.62681658
6	-3.63176873	0.85354348	-1.88215046	6	1.26992763	1.0688499	2.6886721
6	-3.52696665	-0.48524096	-2.17082562	6	0.8191929	2.33558177	2.19027493
6	-2.63867498	-1.04432797	-3.28286221	6	1.5456629	2.99858153	1.19915208
6	-1.97186668	-2.24009143	-2.54671115	6	0.95672549	3.95893498	0.12752875
6	-2.68857004	-2.49039732	-1.3539836	6	1.76399124	3.52440168	-1.09779247
6	-2.05730439	-3.11989167	-0.27255656	6	1.20917865	3.30597272	-2.3338443
6	-2.36542535	-2.70377053	1.07544991	6	1.78030909	2.3191196	-3.20062339
6	-3.31090239	-1.70340038	1.31050779	6	2.94134284	1.62002958	-2.85431854
6	-3.01633063	-0.69942047	2.29692724	6	3.05240832	0.20249383	-3.15914904
6	-3.49339627	0.56178918	1.79989826	6	3.70326689	-0.44497772	-2.05374292
6	-2.71527048	1.70061742	2.02603068	6	3.25807405	-1.71554157	-1.65796008
6	-2.51253635	2.66602977	0.97062203	6	3.10347924	-2.02678431	-0.25577735
6	-3.07896614	2.44867666	-0.29222373	6	3.39480999	-1.05202081	0.71055195
6	-2.36994365	2.81495397	-1.45895072	6	2.55143099	-0.93007561	1.8551961
6	-2.88395343	1.94705774	-2.64655727	6	2.43498492	0.51107701	2.16397517
6	-1.67848124	1.36764941	-3.3868685	6	3.21495997	1.21271702	1.19889624
6	-1.56269183	-0.04063557	-3.68716956	6	2.75235873	2.44220024	0.70595868
6	-0.32912377	-0.57059983	-4.05919562	6	2.90784021	2.76201532	-0.69295625
6	0.15175297	-2.03409392	-3.82932616	6	3.52432683	1.84678311	-1.56038306
6	-0.63740733	-2.63057274	-2.66186311	6	3.9870915	0.567716	-1.05183423
6	0.01134563	-3.27763958	-1.5447713	6	3.82960686	0.26314435	0.30006422
6	-0.70051191	-3.51223586	-0.36647808	6	-3.52283142	-1.47642213	-4.48964305
6	-0.10149853	-3.57045819	1.0722148	6	0.10263618	-2.91654864	-5.14667827
6	-1.17105456	-2.79601437	1.84999502	6	1.99974201	-4.85651151	-1.8351756
6	-0.88414046	-1.83765179	2.7965965	6	0.02482622	-4.9985175	1.69980015
6	-1.79398307	-0.75115921	3.00333033	6	-0.66329443	3.89231131	3.56299858
6	-1.0698119	0.44383903	3.2977301	6	1.234072	5.4829368	0.44553561
6	-1.52668986	1.6493087	2.81509409	6	-0.52265076	4.77697137	-3.43946627
6	-0.605677	2.8153848	2.43973914	6	-3.89541856	2.7132267	-3.59596509
6	-1.23269213	3.25800731	1.08791969	8	0.75074759	0.33587495	4.89437813
6	-0.52942287	3.64209155	-0.05511857	6	2.9196461	-1.64857662	7.98005053
6	-1.1137616	3.41088092	-1.35612371	6	3.60081512	-1.49177254	6.77084394
6	-0.28295858	3.46462171	-2.6355197	6	2.88818366	-1.43912984	5.57933036
6	-0.54758474	2.17936897	-3.46944189	7	1.54295856	-1.4935218	5.59970363
6	0.69615202	1.63363287	-3.86314847	6	0.85364614	-1.68303345	6.74048872
6	0.80413386	0.26843131	-4.15894429	6	1.52679541	-1.74915613	7.95365495
6	1.99947218	-0.45809872	-3.80081426	1	3.46398474	-1.70389874	8.92137213
6	1.60753757	-1.78364654	-3.43100714	1	4.68636409	-1.41883434	6.7318557
6	2.22793307	-2.40333749	-2.37580562	1	3.35356391	-1.33158039	4.60306823
6	1.530006	-3.41360471	-1.46246803	1	-0.22576412	-1.73975005	6.63668453
6	2.01420542	-2.91543524	-0.07110444	1	0.94648127	-1.87595587	8.86595942
6	1.23031693	-2.83151737	1.083858	8	0.85621556	-2.25850333	4.3528396
6	1.50638645	-1.83023996	2.07613276				
6	0.53163152	-1.52842632	3.20694945				

Transition state TS1c, C₇₀(CF₃)₈(O)₂...O...Py

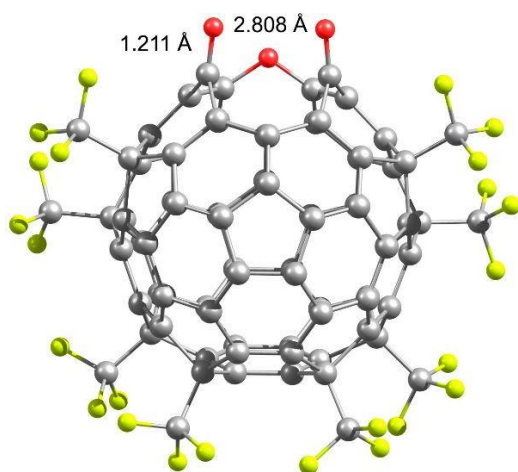


N	X	Y	Z
6	0.18148843	2.45275655	2.16826295
6	1.5699371	2.34132988	2.02879769
6	2.47774998	1.58387604	2.978091
6	0.63621089	-0.34887791	3.9145267
6	-0.60943189	0.03380883	3.19990458
6	-0.92426651	1.4604448	2.9389945
6	-2.10949118	1.62058155	2.01704128
6	-1.92211809	2.69811384	1.09134742
6	-0.55732687	3.1564738	1.17513019
6	0.0918039	3.64345069	0.02936901
6	1.47468276	3.41425299	-0.17347535
6	2.19733004	2.74607068	0.8038623
6	3.54181911	2.14190747	0.42221738
6	3.73027457	0.76911371	1.10324388
6	3.0829787	0.39016332	2.26961996
6	2.71306564	-1.00333027	2.46940721
6	1.45274698	-1.34050135	3.11932669
6	0.72840367	-2.42976547	2.66761878
6	-0.80695909	-2.45076104	2.65838569
6	-1.3558604	-1.02902656	2.62454423
6	-2.52598129	-0.81999546	1.91191306
6	-2.86456238	0.52327083	1.58641483
6	-3.54424346	0.53957925	0.31360874
6	-3.43054405	1.64475803	-0.53806548
6	-2.59518717	2.75480731	-0.13981717
6	-1.91466009	3.2404302	-1.32494605
6	-0.5883691	3.67599211	-1.24151352

N	X	Y	Z
6	0.36914736	3.37350227	-2.26168119
6	1.78605961	3.42914421	-1.69043091
6	2.57847631	2.169515	-2.03991104
6	3.47692799	1.70326325	-1.07462708
6	3.99403996	0.39102159	-1.17601047
6	4.15920104	-0.17560155	0.14147512
6	3.97551757	-1.53354378	0.3671202
6	3.23131568	-1.94761918	1.52762102
6	2.48915681	-3.11822187	1.13834388
6	1.21685492	-3.30065072	1.66596543
6	0.11637281	-3.71623463	0.82869001
6	-1.08241524	-3.12180452	1.28344446
6	-2.06558466	-2.73829699	0.3682025
6	-3.15117418	-1.78867186	0.88519516
6	-3.56646111	-0.79914798	-0.20005572
6	-3.37587151	-1.01485399	-1.54165051
6	-3.16852337	0.10324691	-2.41161374
6	-3.24094037	1.42050483	-1.94674234
6	-2.301015	2.41365049	-2.43549892
6	-1.32706817	2.05460689	-3.3749152
6	0.0079297	2.56460459	-3.30961311
6	0.97489215	1.61371339	-4.01921441
6	2.19184214	1.31338434	-3.13863122
6	2.71796626	0.02329749	-3.22096568
6	3.62413833	-0.4398099	-2.23967229
6	3.45638539	-1.85891286	-2.02374369
6	3.64767837	-2.40439383	-0.74801291
6	2.72305299	-3.38606413	-0.2693153
6	1.65643274	-3.77033474	-1.0932354
6	0.33170316	-3.9297825	-0.5375668
6	-0.64982105	-3.54141681	-1.47711312
6	-1.83900823	-2.95496487	-1.04251108
6	-2.6785767	-2.25497964	-2.1096162
6	-1.73397558	-1.59870707	-3.15583363
6	-2.15733038	-0.2667303	-3.37338135
6	-1.25245742	0.69196845	-3.84659225
6	0.09144524	0.33356428	-4.10278192
6	0.51670243	-0.97770483	-3.90125666
6	2.02567367	-1.20636789	-3.87221575
6	2.39749121	-2.30550725	-2.87528211
6	1.50840427	-3.24547693	-2.41475524
6	0.04405361	-3.31440534	-2.85320439
6	-0.41626178	-1.97075276	-3.41972679
6	4.7497838	3.06139565	0.80117675
9	5.00606828	2.96666218	2.13467076
9	5.87382911	2.68302069	0.13912161

N	X	Y	Z	N	X	Y	Z
9	4.52572286	4.3671459	0.53978258	9	3.94180397	-1.73289123	-5.22285288
6	-1.32888372	-3.25242658	3.8834778	9	2.04780333	-2.71519071	-5.73702158
9	-0.82624934	-2.7317639	5.03971731	6	-0.15014368	-4.52397924	-3.86042004
9	-2.67688224	-3.22992878	3.99072453	9	-0.66504058	-5.61014301	-3.22845864
9	-0.93865228	-4.55245173	3.81876117	9	-0.96382188	-4.20831246	-4.89402123
6	2.49666162	4.72518673	-2.19422961	9	1.03805678	-4.91217177	-4.39448142
9	1.92586027	5.83064429	-1.64816566	8	0.99873994	0.09385582	5.00058921
9	3.81628451	4.74726143	-1.90306678	8	2.76212682	1.96999002	4.08990693
9	2.38994675	4.82965336	-3.54415763	6	-3.19636847	2.28650244	7.75968285
6	-4.42217485	-2.54687233	1.44269522	6	-1.99306735	1.58429798	7.66897064
9	-4.14633293	-3.82582129	1.79539971	6	-1.3065714	1.56429394	6.45337258
9	-4.93080825	-1.91199167	2.53216337	7	-1.82652384	2.20124381	5.40077988
9	-5.4192505	-2.59508729	0.52046359	6	-2.96282296	2.90256415	5.44885299
6	1.35274887	2.19637877	-5.44580472	6	-3.68962732	2.95690639	6.63680603
9	1.06916004	3.52195736	-5.52766383	1	-3.74464603	2.31850202	8.70121985
9	2.66983945	2.05395329	-5.72535786	1	-1.57564865	1.05688439	8.52551183
9	0.64065314	1.58742273	-6.42913217	1	-0.35905097	1.04549074	6.27478112
6	-3.72559643	-3.20850835	-2.75671814	1	-3.26875354	3.40805643	4.53373109
9	-4.61125377	-3.65492908	-1.83249346	1	-4.62004745	3.52163931	6.67291797
9	-4.42770513	-2.5655887	-3.72744069	8	-0.74605904	2.42859729	3.97440043
9	-3.14893949	-4.29637364	-3.31868554				
6	2.59456854	-1.56127597	-5.27749987				
9	2.33939683	-0.60075247	-6.1944959				

Compound 2a, $C_s-C_{70}(CF_3)_8(O)_3$

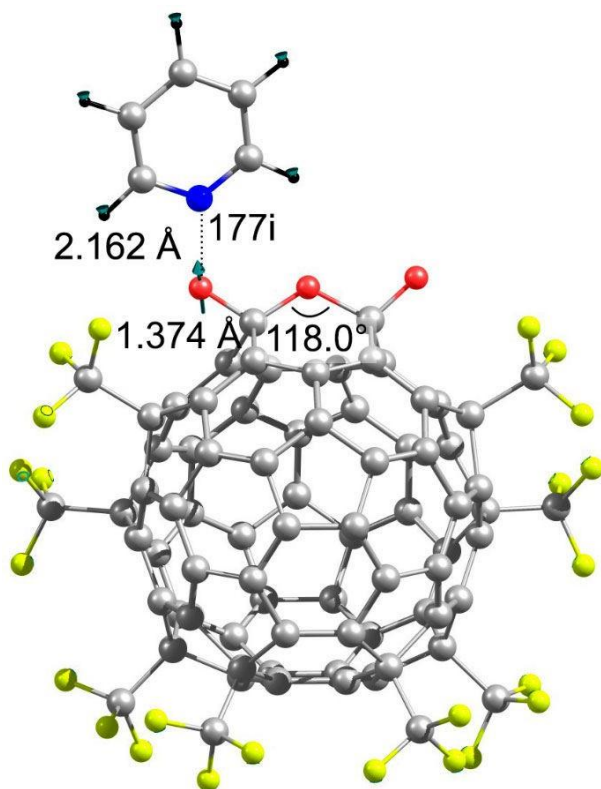


N	X	Y	Z
6	-1.16080954	1.004819	3.95583833
6	-0.05395016	1.84205267	3.80555266
6	1.28183042	1.36895271	4.34886505
6	1.28441056	-1.69035445	4.23662541
6	-0.05414928	-2.09838536	3.65480482

N	X	Y	Z
6	-1.15948936	-1.27333562	3.86854304
6	-2.29751938	-1.33132343	3.0229871
6	-2.99146302	-0.08857094	2.70264441
6	-2.2980174	1.12773127	3.11618166
6	-2.34717474	2.26675752	2.27788796
6	-1.23487258	3.13666682	2.121932
6	-0.07069021	2.87135418	2.82080307
6	1.25377623	3.3789912	2.29042264
6	2.31952516	2.25714059	2.36530421
6	2.2643461	1.15895818	3.2126606
6	2.86652708	-0.1089057	2.7904379
6	2.2729851	-1.40733057	3.12120974
6	2.32817021	-2.44161278	2.19563145
6	1.24247073	-3.53210684	2.02475187
6	-0.07410707	-3.04587488	2.59194472
6	-1.23640545	-3.25327415	1.87743182
6	-2.3497116	-2.40431872	2.10236196
6	-3.14486933	-2.33388405	0.91166467
6	-3.87837951	-1.17952877	0.64634902

N	X	Y	Z	N	X	Y	Z
6	-3.79860796	-0.04718033	1.5505094	6	1.2564796	1.65289382	-3.10279321
6	-3.87578838	1.14801639	0.73264049	6	2.41862581	0.78522444	-2.61620561
6	-3.1367102	2.27636651	1.08166657	6	2.4180053	-0.58678719	-2.66891455
6	-2.46695287	3.07568552	0.10243984	6	1.25926798	-1.4137927	-3.23046807
6	-1.32706448	3.85338114	0.75254915	6	-0.03555785	-0.59968983	-3.22805296
6	-0.01690075	3.63989477	-0.01204283	6	1.79876042	4.61390488	3.07897676
6	1.15603586	3.55926958	0.74576202	9	2.19959085	4.22132951	4.31997034
6	2.32689142	3.01738715	0.16561672	9	2.87370539	5.15431825	2.44907001
6	3.04297612	2.241993	1.15020115	9	0.88029684	5.58555608	3.24856265
6	3.7711157	1.11911556	0.79100314	6	1.70971198	-4.86734948	2.67064742
6	3.66812433	-0.06309002	1.60529841	9	1.94817905	-4.6882458	3.99663518
6	3.77195005	-1.18046252	0.70418936	9	0.77718313	-5.83996301	2.54742666
6	3.04455614	-2.32773368	0.97922548	9	2.85728708	-5.31470877	2.09977225
6	2.3195485	-3.0149866	-0.06251276	6	-1.72371278	5.35810505	0.84647909
6	1.14505635	-3.58767545	0.47558306	9	-2.81907904	5.51402278	1.6352717
6	-0.02852394	-3.6136219	-0.28091743	9	-0.73582834	6.12961305	1.34708788
6	-1.3370812	-3.8893588	0.47111957	9	-2.02557624	5.84463915	-0.38518607
6	-2.47752047	-3.06668135	-0.12210331	6	-1.71824619	-5.42480894	0.52842069
6	-2.47923226	-2.56973115	-1.40045424	9	-0.67362315	-6.22071938	0.2005926
6	-3.18329803	-1.35678692	-1.68361632	9	-2.1385127	-5.77403127	1.77235641
6	-3.92737545	-0.68942174	-0.70288301	9	-2.73215462	-5.71491318	-0.3258756
6	-3.92548666	0.75782858	-0.64900093	6	-1.69207537	4.07425042	-3.19557679
6	-3.18248798	1.49349978	-1.57978621	9	-2.78162842	4.76596156	-2.77254005
6	-2.47174272	2.67718023	-1.20824251	9	-0.68887552	4.96711224	-3.36017612
6	-1.30816854	2.92499407	-2.16920948	9	-2.00994451	3.56010554	-4.41139581
6	-0.01427865	3.19579928	-1.39162024	6	-1.65179023	-3.81417195	-3.43998767
6	1.16038763	2.68890587	-1.94790465	9	-1.87643032	-5.01540667	-2.85028882
6	2.33706415	2.60001604	-1.16882588	9	-2.77285407	-3.4706725	-4.12590452
6	3.12055165	1.45220533	-1.56350207	9	-0.65358737	-3.98506398	-4.33626363
6	3.85179821	0.73644595	-0.60715438	6	1.62179136	2.30161344	-4.47090361
6	3.85122476	-0.69155064	-0.66139612	9	0.66678098	3.15526561	-4.90352678
6	3.12152762	-1.33164355	-1.6711916	9	2.78552109	2.9968406	-4.37649262
6	2.33365932	-2.50231389	-1.36314763	9	1.78107494	1.35055938	-5.42463025
6	1.15565933	-2.52575928	-2.14442827	6	1.64926894	-1.97484391	-4.66094172
6	-0.01752824	-3.06528862	-1.61987941	9	2.08076432	-3.25977648	-4.5791608
6	-1.30714292	-2.73621889	-2.3704016	9	0.61455224	-1.92778418	-5.53054582
6	-1.21118821	-1.29794295	-2.95373494	9	2.66373008	-1.2556008	-5.20761463
6	-2.39551677	-0.59669902	-2.62544797	8	1.53259555	-1.61315448	5.41964095
6	-2.39531148	0.80291007	-2.57410719	8	1.52891772	1.19319497	5.52136919
6	-1.20896755	1.52454541	-2.84405166	8	-1.00295227	-0.16390957	4.69670433
6	-0.03734605	0.84497249	-3.16861622				

Transition state TS1d, C₇₀(CF₃)₈(O)₂...O...Py

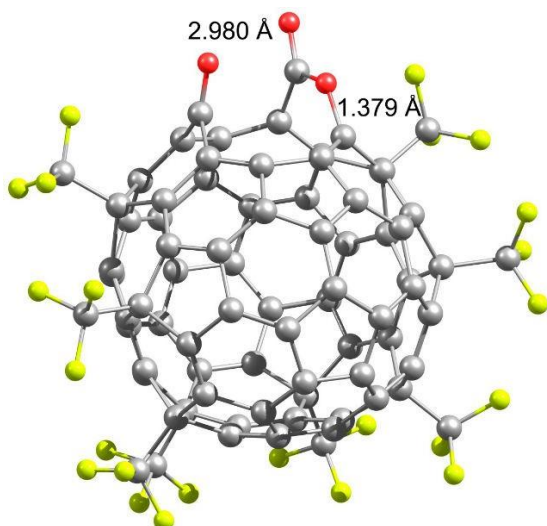


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6	0.60288686	2.8324644	1.70368155
6	1.03243472	2.23353126	3.03244091
6	-0.85276762	0.73228782	3.50746493
6	-1.87324866	0.91806172	2.38136963
6	-1.88890708	2.15188088	1.64993716
6	-2.8172018	2.26202474	0.5591085
6	-2.32133866	3.21251346	-0.40262682
6	-1.04459516	3.66392996	0.08370917
6	-0.00938546	3.89913424	-0.8290471
6	1.3458425	3.57590191	-0.50048737
6	1.6528701	3.06162406	0.74354459
6	3.01801706	2.40332023	0.94390093
6	2.90606523	1.17153928	1.86528636
6	1.88525497	0.99345851	2.77964984
6	1.40841598	-0.34201105	3.05854262
6	-0.0111404	-0.50276893	3.29026367
6	-0.66052979	-1.63150199	2.82209732
6	-2.1190961	-1.64493595	2.31998575
6	-2.55012483	-0.25465741	1.86605485
6	-3.35403647	-0.14040772	0.75731099
6	-3.50587148	1.1251458	0.10900112
6	-3.74643782	0.91994024	-1.29460934
6	-3.27316016	1.8583245	-2.22654187

N	X	Y	Z
6	-2.54588338	3.02745031	-1.7712281
6	-1.47902676	3.2829509	-2.71218157
6	-0.2239622	3.70115946	-2.23753931
6	0.99437369	3.19712547	-2.80518824
6	2.14002531	3.32824739	-1.80354015
6	2.91563972	2.01779785	-1.66863158
6	3.40560454	1.70793884	-0.39860902
6	3.84598497	0.3949528	-0.11741688
6	3.55052874	0.0645972	1.2557629
6	3.22813187	-1.2415655	1.61730485
6	2.1287646	-1.44639614	2.51846307
6	1.44700764	-2.63690905	2.09136288
6	0.05883441	-2.68085301	2.1921836
6	-0.73783327	-3.21346627	1.11225362
6	-1.97321978	-2.53201883	1.04223788
6	-2.58094071	-2.3147053	-0.19694141
6	-3.6982862	-1.27026035	-0.23780673
6	-3.68701694	-0.49185351	-1.55343117
6	-3.07822532	-0.94395332	-2.69938011
6	-2.51660387	0.00302865	-3.61453775
6	-2.64621744	1.38435632	-3.42854268
6	-1.5305955	2.26635895	-3.72980055
6	-0.33060518	1.73136504	-4.20473471
6	0.94096536	2.2249652	-3.76958066
6	2.01904116	1.15542176	-3.95686638
6	2.85447977	0.9928615	-2.68537928
6	3.28690631	-0.2993667	-2.38509672
6	3.79029537	-0.60058481	-1.09958423
6	3.46787841	-1.96160465	-0.73371611
6	3.20210568	-2.28186939	0.6035013
6	2.09921629	-3.14839008	0.89860059
6	1.32871966	-3.64780775	-0.15932183
6	-0.11222489	-3.67365426	-0.05273291
6	-0.70789021	-3.4468985	-1.31436097
6	-1.93100729	-2.78217926	-1.40257942
6	-2.32196045	-2.27258976	-2.79061766
6	-1.04016096	-1.81816211	-3.54488908
6	-1.27303194	-0.54451361	-4.10760535
6	-0.19908544	0.3047542	-4.39915679
6	1.12515599	-0.10848192	-4.13257164
6	1.36709993	-1.3724633	-3.59304151
6	2.7631895	-1.61362671	-3.02862008
6	2.7120578	-2.53250798	-1.80541305
6	1.65589011	-3.36566824	-1.52196371
6	0.40890854	-3.48151002	-2.40066678
6	0.26180021	-2.25032047	-3.29433699

N	X	Y	Z	N	X	Y	Z
6	4.13464094	3.39077372	1.48441671	6	3.73445323	-2.20152332	-4.09540773
9	4.46098815	3.12402433	2.76856996	9	3.82846878	-1.4141353	-5.19157548
9	5.28309333	3.25320858	0.75723693	9	4.98287583	-2.34779192	-3.58073009
9	3.75292528	4.6843505	1.41492833	9	3.31175475	-3.42129771	-4.51167465
6	-3.06410782	-2.27838786	3.42018069	6	0.44385833	-4.8408286	-3.20973438
9	-2.45437016	-2.30632919	4.64023773	9	-0.2362195	-5.81550973	-2.55142827
9	-4.21973715	-1.59398953	3.57363803	9	-0.08787248	-4.71562535	-4.44835958
9	-3.3714162	-3.56692041	3.12054206	9	1.71559605	-5.28772757	-3.36562068
6	3.05924827	4.52049694	-2.20020223	8	-0.14342681	1.87486154	3.85023819
9	2.34094246	5.67094997	-2.29341044	8	1.61531879	3.29185603	3.57081632
9	4.04935864	4.72279638	-1.30411533	6	-1.58848922	1.03917894	9.07549027
9	3.64049916	4.2967987	-3.40671897	6	-0.82287714	1.87661124	8.26254365
6	-5.1151887	-1.8587332	0.04282146	6	-0.8291159	1.66945149	6.88033653
9	-5.15238373	-2.54152957	1.21140212	7	-1.54310652	0.67311461	6.34646815
9	-6.03555648	-0.85886072	0.11827968	6	-2.29666729	-0.13099737	7.09928335
9	-5.51113056	-2.70605409	-0.93292377	6	-2.3397223	0.01962405	8.4873474
6	2.88376637	1.49591945	-5.24130309	1	-1.60570788	1.18385174	10.15605338
9	2.77219991	2.80917142	-5.57130299	1	-0.22731671	2.68779527	8.68000225
9	4.19950799	1.24371266	-5.05864286	1	-0.26308221	2.29238511	6.18545285
9	2.45810924	0.78587776	-6.318672	1	-2.8646161	-0.90224294	6.57812426
6	-3.14672411	-3.3083912	-3.62442107	1	-2.95581255	-0.65125972	9.08514028
9	-4.4267743	-3.38768262	-3.19268871	8	-2.01614663	0.68013959	4.2370054
9	-3.18299422	-2.94178922	-4.93411638				
9	-2.62035729	-4.55246818	-3.55383318				

Compound 5, ester C₇₀(CF₃)₈(O)₃

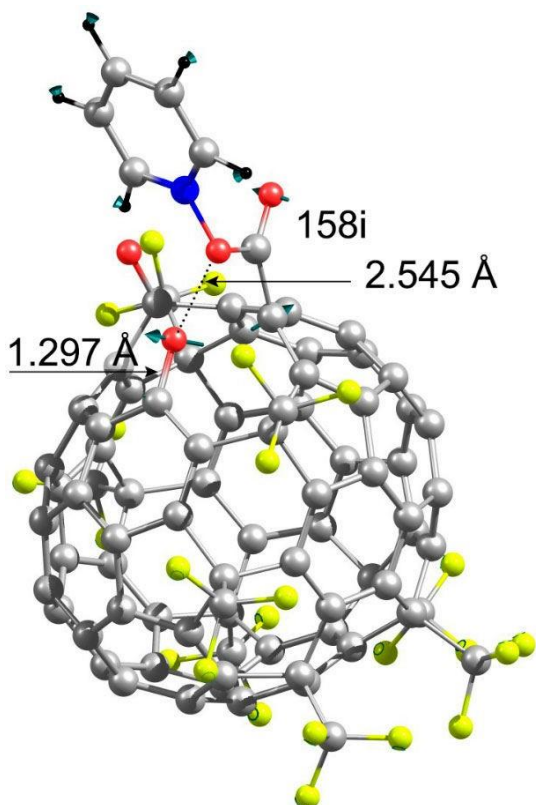


N	X	Y	Z
6	-0.82772728	3.22276504	2.0814049
6	0.54067998	3.05149114	2.39878825

N	X	Y	Z
6	0.99632704	2.44626258	3.7068857
6	-0.70963249	0.60319255	5.18239375
6	-2.12648771	1.23471379	3.29052704
6	-2.01191857	2.36060335	2.44673285
6	-2.90219908	2.40914348	1.33707223
6	-2.41834982	3.3182312	0.33890548
6	-1.13178549	3.77475376	0.7878794
6	-0.12659281	4.00045036	-0.16674024
6	1.2248649	3.70253422	0.12553769
6	1.5458557	3.22063789	1.38902576
6	2.90297324	2.55290609	1.56853066
6	2.81011377	1.34927955	2.52460691
6	1.84160786	1.21175048	3.50595552
6	1.40240444	-0.12176797	3.89075092
6	0.01173362	-0.32902949	4.2765116
6	-0.70606106	-1.37311251	3.71265283
6	-2.19977205	-1.38052262	3.25581541
6	-2.6942994	0.00535989	2.79325125

N	X	Y	Z	N	X	Y	Z
6	-3.47915459	0.05988986	1.64586319	6	1.13127411	-1.35712223	-2.78918201
6	-3.65203369	1.28716159	0.95966338	6	2.54201447	-1.58562456	-2.25413709
6	-3.9138679	1.04183311	-0.43793287	6	2.5204903	-2.45740202	-0.99810506
6	-3.45720415	1.94265001	-1.41138259	6	1.46722337	-3.26963227	-0.65500845
6	-2.69661405	3.11068467	-1.01001442	6	0.19675193	-3.41321004	-1.49515629
6	-1.65498556	3.33551778	-1.99237502	6	0.02741793	-2.2183449	-2.43242814
6	-0.38947859	3.76359777	-1.56922056	6	3.97287902	3.54271579	2.13731183
6	0.8072605	3.24042667	-2.15542746	9	3.73445955	3.75918607	3.46119103
6	1.98359106	3.40001361	-1.1920214	9	5.2223594	3.02673085	2.02021258
6	2.75046505	2.08993454	-1.02935825	9	3.95463276	4.74940066	1.53504273
6	3.27960824	1.82655412	0.23803543	6	-3.09526872	-1.99584248	4.36965996
6	3.72269569	0.52116137	0.55268528	9	-2.96914847	-1.27897633	5.51834021
6	3.46033707	0.23308874	1.94267197	9	-4.40385421	-1.99750247	4.03231271
6	3.14202614	-1.05532896	2.35541508	9	-2.72939661	-3.27493365	4.63916767
6	2.07929804	-1.22294984	3.30568599	6	2.90629879	4.55839735	-1.69344056
6	1.37064509	-2.41637885	2.93187956	9	2.28358589	5.75782893	-1.56494728
6	-0.01456609	-2.42084051	3.05254497	9	4.08003932	4.6185415	-1.02764891
6	-0.84772084	-2.98181761	2.0288858	9	3.20647626	4.38577615	-3.00655871
6	-2.0793241	-2.29400885	1.98312753	6	-5.27110025	-1.72335662	1.00352616
6	-2.71540554	-2.12547032	0.74966991	9	-5.18197935	-2.94202823	1.58513198
6	-3.84482729	-1.10395749	0.69574541	9	-5.9869503	-0.9132153	1.82479443
6	-3.86413146	-0.37346213	-0.64797408	9	-5.99646478	-1.87191011	-0.13349691
6	-3.28465579	-0.86628502	-1.7893499	6	2.6164562	1.42505264	-4.58664817
6	-2.74641193	0.03986911	-2.7593493	9	2.45903285	2.70607754	-5.00724741
6	-2.8611003	1.4262934	-2.61285062	9	3.94271183	1.22312021	-4.40944418
6	-1.74639485	2.28907472	-2.97253654	9	2.19460815	0.62874979	-5.60192066
6	-0.56242072	1.73123705	-3.46599243	6	-3.42005746	-3.26944284	-2.55324225
6	0.72131937	2.23380112	-3.08424726	9	-4.58117653	-3.45200128	-1.8755965
6	1.78657445	1.14993811	-3.26132892	9	-3.73157737	-2.87749968	-3.81561569
6	2.65652618	1.02973195	-2.00710099	9	-2.80693804	-4.4722109	-2.63146258
6	3.09227824	-0.25307997	-1.6726071	6	3.48154797	-2.22628607	-3.31944924
6	3.63257158	-0.50928295	-0.39213242	9	3.58303659	-1.46993904	-4.43503152
6	3.31221046	-1.85501024	0.0299593	9	4.73260234	-2.39423819	-2.81688977
6	3.08333139	-2.13032611	1.38282329	9	3.01681721	-3.44392682	-3.69477303
6	1.98414031	-2.97658505	1.74151856	6	0.21459271	-4.80863284	-2.24714443
6	1.17698264	-3.50172497	0.72569141	9	-0.50501416	-5.7369087	-1.56606881
6	-0.26021707	-3.50685546	0.87193742	9	-0.27951783	-4.72237257	-3.50265652
6	-0.88681654	-3.3262756	-0.37921705	9	1.48009144	-5.29116533	-2.34884683
6	-2.10067824	-2.64630411	-0.45172501	8	-0.50066635	0.68452632	6.36065411
6	-2.53672741	-2.19900964	-1.84544206	8	0.69116019	2.91706028	4.7864589
6	-1.27939855	-1.79051562	-2.66590292	8	-1.70162316	1.37010263	4.59551889
6	-1.52052651	-0.53204716	-3.26435938				
6	-0.44778418	0.29912799	-3.6132068				
6	0.88102263	-0.11325483	-3.36441224				

Transition state TS2d, C₆₉O(CF₃)₈(O)...CO₂Py

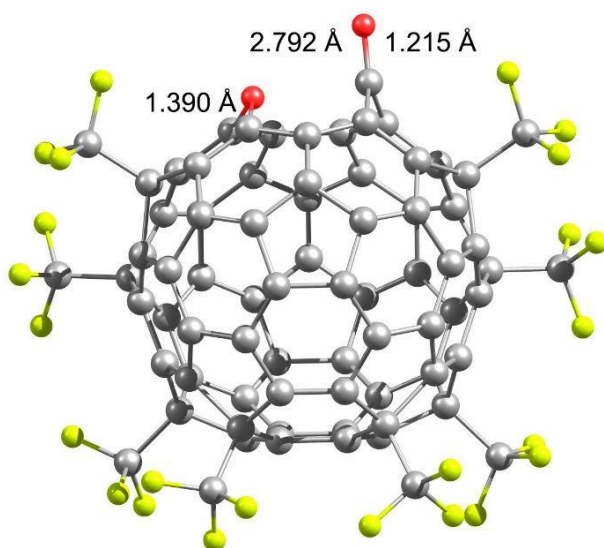


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6	1.73910285	1.96268889	2.74498826
6	0.13385674	-0.08694773	5.03724752
6	-1.40658054	1.56824954	2.26773987
6	-1.14783577	2.69850187	1.44519426
6	-2.03982568	3.00284341	0.38727777
6	-1.33073768	3.70598941	-0.65239365
6	0.04698902	3.77865296	-0.23805727
6	1.06183186	3.67028559	-1.19890009
6	2.27119507	2.99898724	-0.89406837
6	2.45687521	2.48090015	0.38542302
6	3.56248139	1.45505234	0.57835369
6	3.13226519	0.35727941	1.57000446
6	2.16042324	0.51911573	2.55618265
6	1.40310042	-0.62904484	2.99404421
6	0.03223098	-0.46924527	3.59068372
6	-0.99099052	-1.25711998	2.95255307
6	-2.4045531	-0.82241985	2.42385468
6	-2.4378498	0.61108498	1.88678959
6	-3.23327312	0.89461776	0.77972825
6	-3.07132426	2.10805799	0.05409348
6	-3.4064525	1.89989825	-1.33091421
6	-2.7379605	2.60757616	-2.34481572

N	X	Y	Z
6	-1.67269904	3.52557257	-1.99294662
6	-0.62256052	3.40467154	-2.98627412
6	0.72068855	3.46903101	-2.58969367
6	1.70764401	2.60336333	-3.16019126
6	2.89265268	2.44859306	-2.20519483
6	3.25549744	0.97953729	-2.00529488
6	3.70179735	0.6137882	-0.73195744
6	3.7588683	-0.75279686	-0.37734537
6	3.43906532	-0.90898511	1.0227682
6	2.77395482	-2.04317234	1.46944596
6	1.72419193	-1.88446639	2.43189364
6	0.71421858	-2.85883018	2.12859882
6	-0.61004686	-2.42422761	2.2593743
6	-1.57600952	-2.75980985	1.2450208
6	-2.56677744	-1.76436804	1.18420491
6	-3.15633594	-1.44931502	-0.04653211
6	-3.94384095	-0.14229791	-0.13017087
6	-3.75994685	0.52169136	-1.49494449
6	-3.37098133	-0.14946893	-2.62310111
6	-2.61745936	0.53452238	-3.63172359
6	-2.33074147	1.8991269	-3.52921687
6	-1.02306347	2.39499137	-3.92699511
6	-0.05564791	1.50735912	-4.40953142
6	1.32361496	1.63390312	-4.05255576
6	2.0329333	0.28631592	-4.20027827
6	2.85092591	-0.03931447	-2.9475419
6	2.90714922	-1.38277908	-2.57331664
6	3.36839484	-1.74393781	-1.28707911
6	2.68616085	-2.9332476	-0.8234998
6	2.40556027	-3.08873774	0.53785037
6	1.11805898	-3.58006685	0.93966922
6	0.18656283	-3.89142763	-0.05948817
6	-1.18428523	-3.46505691	0.10102581
6	-1.75744328	-3.14823488	-1.14720008
6	-2.72982633	-2.15290795	-1.23379317
6	-3.04149018	-1.64199564	-2.63898734
6	-1.73496828	-1.63751438	-3.48592774
6	-1.616106	-0.38034616	-4.12494235
6	-0.35617726	0.09788062	-4.50961264
6	0.80315404	-0.66935484	-4.25650231
6	0.69793978	-1.91555716	-3.64169167
6	1.99386118	-2.5220848	-3.11046286
6	1.74639892	-3.32097922	-1.82981231
6	0.50919413	-3.78447365	-1.44673392
6	-0.76468842	-3.57631116	-2.27003618
6	-0.60006465	-2.41260476	-3.24650354

N	X	Y	Z	N	X	Y	Z
6	4.88187855	2.10171098	1.110407	9	2.99178688	-2.75941387	-5.30480045
9	4.74871307	2.40267548	2.43479095	9	3.86322135	-3.92525997	-3.66941307
9	5.93157612	1.24779953	0.98939346	9	1.90957922	-4.47622956	-4.50270464
9	5.20558688	3.25440569	0.48497651	6	-1.1687857	-4.93230042	-2.97693878
6	-3.49799839	-1.10497333	3.49150388	9	-2.07837791	-5.61811667	-2.23531367
9	-3.38728102	-0.25669723	4.55587649	9	-1.691154	-4.73760153	-4.21079367
9	-4.75350872	-0.96011803	3.01038342	9	-0.09341633	-5.74875713	-3.12800297
9	-3.39335526	-2.37229915	3.97826718	8	1.07744041	-0.25260804	5.75697119
6	4.0999779	3.2755129	-2.74863661	8	1.7573256	2.56507823	3.81349953
9	3.84376263	4.60877174	-2.68142839	8	-0.56370184	1.36486698	3.23196576
9	5.24825381	3.03679154	-2.0756448	6	-0.28186385	2.79040723	8.92288961
9	4.33874374	2.96837103	-4.05102177	6	-1.08984553	1.6523118	9.01452239
6	-5.49419811	-0.3021017	0.16610697	6	-1.32527785	0.89099958	7.88127969
9	-5.81133199	-1.54529327	0.59926951	7	-0.78181155	1.285197	6.70708086
9	-5.91920873	0.59272386	1.09707715	6	0.01495102	2.37420023	6.56743681
9	-6.23597143	-0.07198426	-0.95114366	6	0.2741289	3.14524559	7.69064636
6	2.88579196	0.27685373	-5.53768389	1	-0.08541968	3.39448456	9.80770221
9	3.09361673	1.53785918	-5.99997146	1	-1.53509316	1.34235148	9.95767405
9	4.10461431	-0.28743914	-5.36640517	1	-1.93232892	-0.00975508	7.83855896
9	2.24180239	-0.39399743	-6.52808025	1	0.41326261	2.56612041	5.56602018
6	-4.21793026	-2.42541153	-3.28946062	1	0.91536877	4.01760659	7.58162763
9	-5.3718029	-2.19898918	-2.6066889	8	-1.082227	0.54471259	5.58448149
9	-4.4149598	-2.03030947	-4.5749334				
9	-4.01482705	-3.76303449	-3.295154				
6	2.69881423	-3.42566067	-4.16364288				

Compound 2b, ketoester C₆₉O(CF₃)₈(O)



N	X	Y	Z	N	X	Y	Z
6	-0.46697182	3.53784195	1.75136237	6	-2.21216587	1.83789946	2.68858055
6	0.73583562	3.17933069	2.38813351	6	-1.83408042	2.94892595	1.91389614
6	0.7677043	2.6579068	3.80535663	6	-2.51079161	3.12152512	0.65962951
				6	-1.64456106	3.80024742	-0.26994125
				6	-0.39236431	4.0174866	0.40316501
				6	0.80924531	3.93439891	-0.31945491
				6	1.9756202	3.397101	0.27964848
				6	1.93487331	3.01765963	1.61603089
				6	3.02917621	2.08632827	2.13057996
				6	2.44535762	1.04777704	3.10986637
				6	1.27233607	1.23976523	3.81584141
				6	0.41906532	0.10776286	4.09714598
				6	-1.01423092	0.27776182	3.97595792
				6	-1.83547497	-0.75794737	3.59662267
				6	-3.13716282	-0.52830726	2.82876238
				6	-3.11437863	0.84705758	2.1927185
				6	-3.6814884	0.99433623	0.93541157
				6	-3.40569295	2.15217415	0.17491835
				6	-3.43595256	1.82347505	-1.23147878

N	X	Y	Z	N	X	Y	Z
6	-2.59736888	2.49649935	-2.12928878	6	1.97918147	-2.99342231	-0.13568447
6	-1.68515345	3.50953075	-1.63428892	6	0.72207714	-3.52549625	0.00992221
6	-0.44433757	3.4018137	-2.37832558	6	-0.34489587	-3.49193915	-1.08534721
6	0.7793148	3.5994035	-1.72436474	6	-0.03970641	-2.39514153	-2.10567659
6	1.91556876	2.77264924	-2.00121191	6	4.17907155	2.85712502	2.85699164
6	2.88406886	2.78669724	-0.81796453	9	3.75518907	3.25101646	4.08985466
6	3.27457886	1.36836857	-0.40304594	9	5.2648135	2.06014837	3.02780002
6	3.46460489	1.14202263	0.96413673	9	4.57022026	3.970583	2.20366968
6	3.50272195	-0.18624273	1.45278577	6	-4.34753635	-0.70872612	3.78929625
6	2.89447289	-0.24882564	2.75970404	9	-4.21477088	0.12083504	4.85953896
6	2.19147018	-1.37668335	3.17310538	9	-5.52674945	-0.41871867	3.19506089
6	0.92932992	-1.19939505	3.84249365	9	-4.41337398	-1.98168229	4.25565352
6	0.07265867	-2.27489659	3.41754049	6	4.13189279	3.65196377	-1.185325
6	-1.28304953	-2.01902047	3.24676196	9	3.79000867	4.96029325	-1.30703459
6	-1.99288886	-2.51664378	2.09027276	9	5.12134104	3.55837818	-0.27061538
6	-3.00279861	-1.60052801	1.70859205	9	4.65243153	3.24724778	-2.3727077
6	-3.30250796	-1.41041314	0.35765834	6	-5.67902082	-0.40954748	0.01282252
6	-4.1174254	-0.16195681	0.00009319	9	-6.0187222	-1.49090622	0.75188441
6	-3.68222169	0.41497669	-1.34806582	9	-6.33490243	0.66927048	0.51475103
6	-3.00958455	-0.30994411	-2.29969326	9	-6.15516073	-0.61373175	-1.24064079
6	-2.08930209	0.35262957	-3.17485116	6	3.70220387	0.35270744	-3.85286382
6	-1.90732027	1.73890015	-3.13774231	9	3.92144011	1.57954754	-4.39155719
6	-0.57533012	2.30038352	-3.29175557	9	4.88683299	-0.08994949	-3.37134497
6	0.5223885	1.45405857	-3.48080594	9	3.32714691	-0.45745591	-4.87558874
6	1.78487964	1.70984168	-2.85872573	6	-3.52469634	-2.69748639	-2.95746379
6	2.58284052	0.41084499	-2.72801464	9	-4.81209137	-2.58455974	-2.5467841
6	3.13012798	0.24846903	-1.30681643	9	-3.47620536	-2.36031471	-4.27247916
6	3.17501541	-1.05200134	-0.80274621	9	-3.18107663	-4.00131057	-2.85143444
6	3.3644541	-1.27223101	0.5804159	6	3.42414056	-3.23416204	-2.1903478
6	2.6558991	-2.45840671	1.00567577	9	3.93471276	-2.64289925	-3.2937039
6	2.09332499	-2.52368873	2.2862864	9	4.46571083	-3.61635839	-1.40593688
6	0.78148564	-3.07804476	2.43695427	9	2.77377096	-4.35427945	-2.59329644
6	0.10763914	-3.54405785	1.30143917	6	-0.48677838	-4.93333139	-1.7318765
6	-1.29544231	-3.24817179	1.12096875	9	-1.54116084	-5.60418067	-1.20104159
6	-1.58957187	-3.06708003	-0.25029483	9	-0.64672895	-4.8812155	-3.07364464
6	-2.57715908	-2.1633581	-0.64058216	9	0.61739064	-5.68703583	-1.49096303
6	-2.59432722	-1.77268113	-2.11662091	8	0.49385936	3.32780101	4.78114847
6	-1.13544805	-1.72737227	-2.65181743	8	-1.46896127	1.58364753	3.83307792
6	-0.95262801	-0.51796936	-3.36147194				
6	0.33042899	0.02317682	-3.51233153				
6	1.44868266	-0.63342982	-2.94986896				
6	1.28196429	-1.83118486	-2.258132				
6	2.46114944	-2.29325945	-1.4069241				

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